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Microlocal Analysis, Sharp Spectral Asymptotics and Applications V

Applications to Quantum Theory and Miscellaneous Problems

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Preface

The Problem of the *Spectral Asymptotics*, in particular the problem of the *Asymptotic Distribution of the Eigenvalues*, is one of the central problems in the *Spectral Theory of Partial Differential Operators*; moreover, it is very important for the *General Theory of Partial Differential Operators*.

I started working in this domain in 1979 after R. Seeley [1] justified a remainder estimate of the same order as the then hypothetical second term for the Laplacian in domains with boundary, and M. Shubin and B. M. Levitan suggested me to try to prove Weyl's conjecture. During the past almost 40 years I have not left the topic, although I had such intentions in 1985, when the methods I invented seemed to fail to provide the further progress and only a couple of not very exciting problems remained to be solved. However, at that time I made the step toward local semiclassical spectral asymptotics and rescaling, and new much wider horizons opened.

So I can say that this book is the result of 40 years of work in the Theory of Spectral Asymptotics and related domains of Microlocal Analysis and Mathematical Physics (I started analysis of *Propagation of singularities* (which plays the crucial role in my approach to the spectral asymptotics) in 1975).

This monograph consists of five volumes. This Volume II concludes the general theory. It consists of two parts. In the first one we develop methods of combining local asymptotics derived in Volume I, with estimates of the eigenvalue counting functions in the small domains (singular zone) derived by methods of functional analysis. In the second part we derive eigenvalue asymptotics which either follow directly from the general theory, or require applications of the developed methods (if the operator has singularities or degenerations, strong enough to affect the asymptotics).

Victor Ivrii,
Toronto, June 10, 2019.

Contents

Introduction

This Volume is devoted to applications. In Part XI we consider Multiparticle Quantum Theory, and in Part XII Miscellaneous problems (again, including Multiparticle Quantum Theory).

Part XI. Asymptotics of the Ground State Energy of Heavy Atoms and Molecules

In this Part we consider an application to Thomas-Fermi Theory. Consider a large (heavy) atom or molecule; it is described by *Multiparticle Quantum Hamiltonian*

$$\mathsf{H}_N = \sum_{1\le n\le N} H_V(x_n) + \sum_{1\le n<k\le N} \frac{1}{|x_n - x_k|}, \tag{0.1}$$

where H is *one-particle quantum Hamiltonian*, Planck constant $\hbar = 1$, electron mass $= \frac{1}{2}$, electron charge $= -1$, y_m is a location of m-th nuclei and Z_m its charge, M is fixed, but $Z_m \asymp N \to \infty$.

This operator acts on the space $\wedge_{1\le j\le N}\mathscr{L}^2(\mathbb{R}^3, \mathbb{C}^2)$ of totally antisymmetric functions $\Psi(x_1, \varsigma_1; \dots; x_N, \varsigma_N)$ because electrons are Fermions, $x_n = (x_n^1, x_n^2, x_n^3)$ is a coordinate and $\varsigma_n \in \{-\frac{1}{2}, \frac{1}{2}\}$ is a *spin* of n-th particle. We identify $\mathbb{C}^2$-valued function $\psi(x)$ on $\mathbb{R}^3$ with scalar-valued $\psi(x, \varsigma)$

If electrons were not interacting between themselves, but the field potential was $-W(x)$, then they would occupy lowest eigenvalues and ground state wave functions would be (anti-symmetrized) $\phi_1(x_1, \varsigma_1)\phi_2(x_2, \varsigma_2)\dots\phi_N(x_N, \varsigma_N)$ where ϕ_n and λ_n are eigenfunctions and eigenvalues of H_W.

Then the local electron density would be $\rho_\Psi = \sum_{1\le n\le N} |\phi_n(x)|^2$ and according to pointwise Weyl law (if there is no magnetic field)

$$\rho_\Psi(x) \approx \frac{1}{3\pi^2}(W + \nu)_+^{\frac{3}{2}}, \tag{0.2}$$

where $\nu=\lambda_N$; here we assume that $H_V=\Delta-V(x)$ as it is in Chapter 25.

This density would generate potential $-|x|^{-1}*\rho_\Psi$ and we would have $W\approx V-|x|^{-1}*\rho_\Psi$.

Replacing all approximate equalities by strict ones we arrive to Thomas-Fermi equations:

$$V-W^{\mathsf{TF}}=|x|^{-1}*\rho^{\mathsf{TF}}, \tag{0.3}$$

$$\rho^{\mathsf{TF}}=\frac{1}{3\pi^2}(W^{\mathsf{TF}}+\nu)_+^{\frac{3}{2}}, \tag{0.4}$$

$$\int \rho^{\mathsf{TF}}\,dx=N, \tag{0.5}$$

where $\nu\le 0$ is called *chemical potential* and in fact approximates λ_N.

Thomas-Fermi theory has been rigorously justified (with pretty good error estimates).

Chapter 25. No Magnetic Field Case. In this chapter we assume that there is no magnetic field: $H_V=\Delta-V(x)$ with

$$V(x)=\sum_{1\le m\le M}\frac{Z_m}{|x-\mathsf{y}_m|}, \tag{0.6}$$

where y_m is a *position* and Z_m is a *charge* of m-th nuclei, M is fixed and $Z_1\asymp Z_2\asymp\cdots\asymp Z_M\asymp N$.

Section 25.1 is an Introduction and in *Section 25.2* we justify a reduction of the original multiparticle problem to one-particle one. This is done mainly by methods of the classical mathematical physics (functional analysis).

In *Section 25.3* we expose *Thomas-Fermi theory* described by (0.3)–(0.5).

In *Section 25.4* we, based on previous sections and chapters, prove our main results. First of all, the *ground state energy* is given by

$$\begin{aligned}\mathsf{E}_N=2\frac{(6\pi^2)^{\frac{5}{3}}}{15\pi^2}&\int\Bigl(\rho^{\mathsf{TF}\,\frac{5}{3}}-V\rho^{\mathsf{TF}}\Bigr)\,dx\\ &-\frac{1}{2}\iint\rho^{\mathsf{TF}}(x)\rho^{\mathsf{TF}}(y)|x-y|^{-1}\,dxdy+O(Z^2).\end{aligned} \tag{0.7}$$

Using results of Section 12.6 *Riesz Means for Operators with Singularities*, we improve the remainder estimate to $O(Z^{\frac{5}{3}})$ but we need to include the *Scott correction term*

$$\sum_{1\le m\le M}S_0Z_m^2, \tag{0.8}$$

and even to $O(Z^{\frac{5}{3}-\delta})$ but we need to include *Dirac and Schwinger correction terms* $\sim Z^{\frac{5}{3}}$.

In *Section 25.5* we consider *negatively charged systems* (i.e. those with $Z := Z_1 + \ldots + Z_m < N$) and estimate *excessive negative charge* $(N - Z)$, when system is able to bind N electrons, i.e. $\mathsf{E}_N < \mathsf{E}_{N-1}$.

In *Section 25.6* we consider *positively charged systems* (i.e. those with $Z > N$) and estimate or find asymptotics $\mathsf{I}_N \approx \nu_N$ for an *ionization energy* $\mathsf{I}_N := \mathsf{E}_{N-1} - \mathsf{E}_N$.

We also consider systems with free $\mathsf{y}_1, \ldots, \mathsf{y}_M$ and include in the total energy the *internuclear energy*

$$\sum_{1\le m<m'\le M} \frac{Z_m Z_{m'}}{|\mathsf{y}_m - \mathsf{y}_{m'}|}, \tag{0.9}$$

and minimize the ground state energy by $\mathsf{y}_1, \ldots, \mathsf{y}_M$ and recover all afore-mentioned results.

We also estimate *excessive positive charge* $(Z - N)$ for which system does not disintegrate into separate atoms.

Chapter 26. The Case of External Magnetic Field. Here we assume that there is a constant magnetic field with a magnetic potential $\boldsymbol{A}(x) = B(-\frac{1}{2}x_2, \frac{1}{2}x_1, 0)$ and then one-particle Hamiltonian is Schrödinger-Pauli operator:

$$H = ((-ih\nabla - \mu\boldsymbol{A}(x)) \cdot \boldsymbol{\sigma})^2 + V(x) \tag{0.10}$$

(see, f.e. Volume III, (0.41)). We assume that the magnetic field is not hyperstrong: $B \ll N^3$. Still it may be sufficiently strong to affect pointwise Weyl formula, which needs to be modified according to Chapter 13 (the results of Chapter 14 are not needed here).

Basically there are two principally cases $B \ll Z^{\frac{4}{3}}$ of a moderate magnetic field and $Z^{\frac{4}{3}} \ll B \ll Z^3$ of a strong magnetic field and a transitional case.

Section 26.1 is an Introduction (which is parallel to Sections 25.1 and 25.2, arguments and results of which require almost no modification).

Section 26.2 is parallel to Section 25.3 but instead of Section 25.4 we have four *Sections 26.3–26.6*, covering single nucleus case $M = 1$, multiple nuclei case $M \ge 2$ with analysis “inside molecule” and “near the molecule edge”and the synthesis, respectively.

Sections 26.7 and *26.8* are similar to Sections 25.5 and 25.6.

Chapter 27. The Case of Self-Generated Magnetic Field. Here we consider the same Schrödinger-Pauli operator but magnetic field is underdetermined a priory and its energy

$$\alpha^{-1}\int |\nabla \times \mathbf{A}|^2\, dx \tag{0.11}$$

is included in the total energy. Here we assume that $\alpha Z_m \le \kappa^*$ with some constant $\kappa^* > 0$. We recover the same results as in Chapter 25 but with the *Scott correction term*

$$\sum_{1\le m\le M} S(\alpha Z_m) Z_m^2 \tag{0.12}$$

instead of (0.8).

Section 27.1 is an Introduction. *Sections 27.2* and *27.3* provide a replacement for Sections 12.6: while Section 27.2 treats a single singularity, Section 27.3 deals with a molecular case and the necessity to "decouple" singularities.

In *Section 27.4* as in Section 25.4 the asymptotics of the ground state energy is recovered and *Section 27.5* is similar to Sections 25.5 and *Section 25.6.*

Chapter 28. The Case of Combined Magnetic Field. This chapter combines two previous ones: there is an external constant magnetic field $\mathbf{A}_0(x) = B(-\frac{1}{2}x_2, \frac{1}{2}x_1, 0)$ and an unknown self-generated magnetic field $\bigl(\mathbf{A} - \mathbf{A}_0\bigr)(x)$, and the energy of the latter

$$\alpha^{-1}\int |\nabla \times (\mathbf{A} - \mathbf{A}_0(x))|^2\, dx \tag{0.13}$$

should be added to the total energy.

Section 28.1 is an Introduction. Since we need a lot of microlocal arguments, they spread over six sections: *Sections 28.2–28.4* cover the local theory and *Sections 28.5* and *28.6* the global theory under different assumptions.

However applications to the ground state energy, excessive negative and positive charges and ionization energy need only small modifications of our previous arguments and squeeze into a single *Section 28.7.*

Part XII. Articles

I decided to put results of the last few years in this volume as separate articles. So far those are[1)]

- Joint paper with A. Hassel [1] *Spectral asymptotics for the semiclassical Dirichlet to Neumann operator.*

- My paper [29] *Spectral asymptotics for fractional Laplacians.*

- My paper [32] *Spectral asymptotics for Dirichlet to Neumann operator in the domains with edges.*

- My paper [30] *Asymptotics of the ground state energy in the relativistic settings.*

- My paper [31] *Asymptotics of the ground state energy in the relativistic settings and with self-generated magnetic field.*

- My paper [33] *Complete semiclassical spectral asymptotics for periodic and almost periodic perturbations of constant operator.*

- My paper [34] *Complete Differentiable Semiclassical Spectral Asymptotics.*

  item My paper [34] *Bethe-Sommerfeld conjecture in semiclassical settings.*

- My paper [28] *100 years of Weyl's law.*

See also the List of my presentations with links to them.

[1)] While I do not plan to change the main body of this book, I intend to add new articles, as soon as I write them.

Part XI

Application to Multiparticle Quantum Theory

Chapter 25

No Magnetic Field Case

25.1 Introduction

The purpose of this Part is to apply semiclassical methods developed in the previous parts to the theory of heavy atoms and molecules. Because of this we combine our semiclassical methods with the traditional methods of that theory, mainly function-analytic.

In this Chapter we consider the case without magnetic field. Next chapters will be devoted to the cases of the self-generated magnetic field, strong external magnetic field and the combined external and self-generated fields. Basically this Chapter should be considered as an introduction.

We explore the ground state energy, an excessive negative charge, ionization energy and excessive negative charge when atoms can still bind into molecules.

25.1.1 Framework

Let us consider the following operator (quantum Hamiltonian)

$$\mathsf{H} = \mathsf{H}_N := \sum_{1\le j\le N} H_{V,x_j} + \sum_{1\le j<k\le N} |x_j - x_k|^{-1} \tag{25.1.1}$$

on

$$\mathfrak{H} = \bigwedge_{1\le n\le N} \mathsf{H}, \qquad \mathsf{H} = \mathscr{L}^2(\mathbb{R}^d, \mathbb{C}^q) \tag{25.1.2}$$

with

$$H_V = D^2 - V(x) \tag{25.1.3}$$

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describing N same type particles in the external field with the scalar potential $-V$ (it is more convenient but contradicts notations of the previous chapters), and repulsing one another according to the Coulomb law.

Here $x_j \in \mathbb{R}^d$ and $(x_1, \dots, x_N) \in \mathbb{R}^{Nd}$, potential $V(x)$ is assumed to be real-valued. Except when specifically mentioned we assume that

$$V(x) = \sum_{1\le m\le M} \frac{Z_m}{|x - \mathsf{y}_m|} \tag{25.1.4}$$

where $Z_m > 0$ and y_m are charges and locations of nuclei.

Mass is equal to $\frac{1}{2}$ and the Plank constant and a charge are equal to 1 here. The crucial question is the quantum statistics.

(25.1.5) We assume that the particles (electrons) are *fermions*. This means that the Hamiltonian should be considered on the *Fock space* $\mathfrak{H}$ defined by (25.1.2) of the functions antisymmetric with respect to all variables $(x_1, \varsigma_1), \dots, (x_N, \varsigma_N)$.

Here $\varsigma \in \{1, \dots, q\}$ is a *spin variable*.

Remark 25.1.1. (i) Meanwhile for *bosons* one should consider this operator on the space of symmetric functions. The results would be very different from what we will get here. Since our methods fail in that framework, we consider only fermions here.

(ii) In this Chapter we do not have magnetic field and we can assume that $q = 1$; for $q \ge 1$ no modifications of our arguments is required and results are the same albeit with different numerical coefficients. In the next chapters we introduce magnetic field (external or self-generated) we will be interested in $d = 3$, $q = 2$ and

$$H_{V,A} = \bigl((i\nabla - A)\cdot \boldsymbol{\sigma}\bigr)^2 - V(x) \tag{25.1.6}$$

where $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$, σ_k are Pauli matrices.

Let us assume that

(25.1.7) Operator H is self-adjoint on $\mathfrak{H}$.

As usual we will never discuss this assumption.

25.1.2 Problems to Consider

We are interested in the *ground state energy* $\mathsf{E} = \mathsf{E}_N$ of our system i.e. in the lowest eigenvalue of the operator $\mathsf{H} = \mathsf{H}_N$ on $\mathfrak{H}$:

$$\mathsf{E} := \inf \operatorname{Spec} \mathsf{H} \qquad \text{on} \quad \mathfrak{H}; \tag{25.1.8}$$

more precisely we are interested in the asymptotics of $\mathsf{E}_N = \mathsf{E}(\underline{\mathsf{y}}; \underline{Z}; N)$ as V is defined by (25.1.4) and $N \asymp Z := Z_1 + Z_2 + ... + Z_M \to \infty$ and we are going to prove that[1)] E is equal to *Thomas-Fermi energy* $\mathcal{E}^{\mathsf{TF}}$ with Scott and Dirac-Schwinger corrections and with $o(Z^{\frac{5}{3}})$ error.

Here we use notations $\underline{\mathsf{y}} = (\mathsf{y}_1, \dots, \mathsf{y}_M)$, $\underline{Z} = (Z_1, \dots, Z_M)$.

We are also interested in the asymptotics for the *ionization energy*

$$\mathsf{I}_N := \mathsf{E}_{N-1} - \mathsf{E}_N. \tag{25.1.9}$$

It is well-known (see G. Zhislin [1]) that $\mathsf{I}_N > 0$ as $N \leq Z$ (i.e. molecule can bind at least Z electrons) and we are interested in the following question: estimate *maximal excessive negative charge*

$$\max_{N:\ \mathsf{I}_N > 0} (N - Z) \tag{25.1.10}$$

i.e. *how many extra electrons can bind a molecule?*.

All these questions so far were considered in the framework of the fixed positions $\mathsf{y}_1, \dots, \mathsf{y}_M$ but we can also consider

$$\widehat{\mathsf{E}} = \widehat{\mathsf{E}}_N = \widehat{\mathsf{E}}(\underline{\mathsf{y}}; \underline{Z}; N) = \mathsf{E} + U(\underline{\mathsf{y}}; \underline{Z}) \tag{25.1.11}$$

with

$$U(\underline{\mathsf{y}}; \underline{Z}) := \sum_{1 \leq m < m' \leq M} \frac{Z_m Z_{m'}}{|\mathsf{y}_m - \mathsf{y}_{m'}|} \tag{25.1.12}$$

and

$$\widehat{\mathsf{E}}(\underline{Z}; N) = \inf_{\mathsf{y}_1, \dots, \mathsf{y}_M} \widehat{\mathsf{E}}(\underline{\mathsf{y}}; \underline{Z}; N) \tag{25.1.13}$$

and replace I_N by $\widehat{\mathsf{I}}_N = -\widehat{\mathsf{E}}_N + \widehat{\mathsf{E}}_{N-1}$ and modify all our questions accordingly. We call these frameworks *fixed nuclei model* and *free nuclei model* respectively.

In the free nuclei model we can consider two other problems:

[1)] Under reasonable assumption $|\mathsf{y}_m - \mathsf{y}_{m'}| \gg Z^{-\frac{1}{3}}$ for all $m \neq m'$.

(a) Estimate from below *minimal distance between nuclei* i.e.

$$a := \min_{1\le m<m'\le M} |\mathsf{y}_m - \mathsf{y}_{m'}|$$

for which such minimum is achieved;

(b) Estimate *maximal excessive positive charge*

$$\max_N \bigl\{Z - N\colon \widehat{\mathsf{E}} < \min_{\substack{N_1,\dots,N_M:\\ N_1+\dots N_M=N}} \sum_{1\le m\le M} \mathsf{E}(Z_m; N_m)\bigr\} \tag{25.1.14}$$

for which molecule does not disintegrates into atoms[2)].

25.1.3 Thomas-Fermi Theory

The first approximation is the Thomas-Fermi theory. Let us introduce the *spacial density* of the particle with the state $\Psi \in \mathfrak{H}$:

$$\rho(x) = \rho_\Psi(x) = N \int |\Psi(x, x_2, \dots, x_N)|^2\, dx_2 \cdots dx_N \tag{25.1.15}$$

where $|\cdot|$ means a norm in $\mathbb{C}^{Nq}$ and antisymmetricity of Ψ implies that it does not matter what variable x_j is replaced by x while in the general case one should sum on $j = 1, \dots, N$. Let us write the Hamiltonian, describing the corresponding "quantum liquid":

$$\mathcal{E}(\rho) = \int \tau(\rho(x))\, dx - \int V(x)\rho(x)\, dx + \frac{1}{2}\mathsf{D}(\rho, \rho), \tag{25.1.16}$$

with

$$\mathsf{D}(\rho, \rho) = \iint |x - y|^{-1}\rho(x)\rho(y)\, dxdy \tag{25.1.17}$$

where τ is the energy density of a gas of noninteracting electrons. Namely,

$$\tau(\rho) = \sup_{w\ge 0} \bigl(\rho w - P(w)\bigr) \tag{25.1.18}$$

[2)] One can ask the same question about disintegration into smaller molecules but our methods are too crude to distinguish between such questions.

is the Legendre transform of the *pressure* $P(w)$ given by the formula

$$P(w) = \varkappa_1 w_+^{\frac{d}{2}+1}, \qquad \varkappa_1 = 2(2\pi)^{-d}(d+2)^{-1}\varpi_d q. \tag{25.1.19}$$

The classical sense of the second and the third terms in the right-hand expression of (25.1.16) is clear and the density of the kinetic energy is given by $\tau(\rho)$ in the semiclassical approximation (see Remark 25.1.2). So, the problem is

(25.1.20) Minimize functional $\mathcal{E}(\rho)$ defined by (25.1.16) under restrictions:

$$\rho \geq 0, \qquad \int \rho\, dx \leq N. \tag*{(25.1.21)$_{1,2}$}$$

The solution if exists is unique because functional $\mathcal{E}(\rho)$ is strictly convex (see below). The existence and the property of this solution denoted further by ρ^{TF} is known in the series of physically important cases.

Remark 25.1.2. If w is the negative potential then

$$\operatorname{tr} e(x,x,0) \approx P'(w) \tag{25.1.22}$$

defines the density of all non-interacting particles with negative energies at point x and

$$\int_{-\infty}^{0} \tau\, d_\tau \operatorname{tr} e(x,x,\tau) dx \approx -\int P(w)\, dx \tag{25.1.23}$$

is the total energy of these particles; here $\approx$ means "in the semiclassical approximation".

We consider in the case of $d=3$ a large (heavy) molecule with potential (25.1.4). It is well-known[3)] that

Proposition 25.1.3. *(i) For $V(x)$ given by* (25.1.4) *minimization problem* (25.1.20) *has a unique solution $\rho = \rho^{\mathsf{TF}}$; then denote $\mathcal{E}^{\mathsf{TF}} := \mathcal{E}(\rho^{\mathsf{TF}})$;*

(ii) Equality in (25.1.21)$_2$ *holds if and only if $N \leq Z := \sum_m Z_m$.*

3) E. Lieb, "Thomas-fermi and related theories of atoms and molecules", [4], pp. 263–301.

(iii) Further, ρ^{TF} does not depend on N as $N \ge Z$.

(iv) Thus

$$\int \rho^{\mathsf{TF}}\,dx = \min(N, Z), \qquad Z := \sum_{1\le m\le M} Z_m. \tag{25.1.24}$$

25.1.4 Main Results Sketched and Plan of the Chapter

In the first half of the Chapter we derive asymptotics for ground state energy and justify Thomas-Fermi theory.

First of all, in Section 25.2 we reduce the calculation of E to calculation of $\mathsf{N}_1(H_W - \nu)$ and to estimate for $\mathsf{D}\bigl(e(x,x,\nu) - \rho, e(x,x,\nu) - \rho\bigr)$ where $\mathsf{N}_1(H_W - \nu) = \mathsf{Tr}((H_W - \nu)^-)$ is the sum of the negative eigenvalues of operator $H_W - \nu$ $H_W = D^2 - W$, $W = W^{\mathsf{TF}}$, $\rho = \rho^{\mathsf{TF}}$ are Thomas-Fermi potential and Thomas-Fermi density respectively (or their appropriate approximations), ν is either λ_N (N-th eigenvalue of H_W) or its appropriate approximation and $e(x,y,\nu)$ is the Schwartz kernel of $E(\nu)$ which is the spectral projector of H_W.

Section 25.3 is devoted to the systematic presentation of the Thomas-Fermi theory.

Further, in Section 25.4 we apply our standard semiclassical arguments and calculate $\mathsf{N}_1(H_W - \nu)$ and estimate $\mathsf{D}\bigl(e(x,x,\nu) - \rho, e(x,x,\nu) - \rho\bigr)$ and also $|\lambda_N - \nu|$ where now ν is the chemical potential (which is the Thomas-Fermi approximation to λ_N). As a result under appropriate restrictions to N, Z and

$$a := \min_{j\ne k} |\mathsf{y}_j - \mathsf{y}_k| \gg Z^{-\frac{1}{3}} \tag{25.1.25}$$

we prove that

$$\mathsf{E} = \mathcal{E}^{\mathsf{TF}} + \mathsf{Scott} + \mathsf{Dirac} + \mathsf{Schwinger} + o(Z^{\frac{5}{3}}) \tag{25.1.26}$$

and

$$\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}}, \rho_\Psi - \rho^{\mathsf{TF}}) = o(Z^{\frac{5}{3}}) \tag{25.1.27}$$

where

$$\mathsf{Scott} = q \sum_{1\le m\le M} Z_m^2 \tag{25.1.28}$$

$$\mathsf{Dirac} = -\frac{9}{2}(36\pi)^{\frac{2}{3}} q^{\frac{2}{3}} \int (\rho^{\mathsf{TF}})^{\frac{4}{3}}\, dx, \tag{25.1.29}$$

$$\mathsf{Schwinger} = (36\pi)^{\frac{2}{3}} q^{\frac{2}{3}} \int (\rho^{\mathsf{TF}})^{\frac{4}{3}}\, dx \tag{25.1.30}$$

and Ψ is the ground state.

Remark 25.1.4. (i) Actually we will recover even slightly better remainder estimate $O(Z^{\frac{5}{3}-\delta})$ in (25.1.26) and (25.1.27) as $a \ge Z^{-\frac{1}{3}+\delta_1}$.

(ii) Condition $a \gtrsim Z^{-\frac{1}{3}}$ bans nuclei to be so close that the repulsion energy between them be much larger than the total energy of all the electrons. Estimates in case when this condition is violated will be also proven;

(iii) Keeping in mind that there is no binding in Thomas-Fermi theory (and this statement could be quantified) one gets immediately that in the free nuclei model $a \ge Z^{-\frac{5}{21}}$ and therefore remainder estimate $O(Z^{\frac{5}{3}-\delta})$ holds.

(iv) Due to scaling in the Thomas-Fermi theory (see proposition 25.3.3) $\mathcal{E}^{\mathsf{TF}} \sim q^{\frac{2}{3}} Z^{\frac{7}{3}} = q^3 (q^{-1}Z)^{\frac{3}{7}}$, $\mathsf{Scott} \sim qZ^2 = q^3(q^{-1}Z)^2$, and both Dirac and $\mathsf{Schwinger}$ are $\sim q^{\frac{4}{3}} Z^{\frac{5}{3}} = q^3(q^{-1}Z)^{\frac{5}{3}}$.

In the second half of the Chapter we apply estimate (25.1.27) to investigate negatively and positively charged systems. In Section 25.5 we consider negatively charged systems and derive an upper estimate for the excessive negative charge $(N - Z)$ such that $\mathsf{I}_N > 0$ and ionization energy I_N itself.

In Section 25.6 we derive upper and lower estimates for $\mathsf{I}_N + \nu$ and an upper estimate for the excessive positive charge for which in the framework of the free nuclei model $a < \infty$.

25.2 Reduction to Semiclassical Theory

To justify the heuristic formula $\mathsf{E} \sim \mathcal{E}^{\mathsf{TF}} = \mathcal{E}(\rho^{\mathsf{TF}})$ and to find an error estimate let us deduce the lower and upper estimates for E.

25.2.1 Lower Estimate

For the lower estimate we apply the *electrostatic inequality* due to E. H. Lieb:

$$\sum_{1\le j<k\le N}\int |x_j-x_k|^{-1}|\Psi(x_1,\dots,x_N)|^2\,dx_1\cdots dx_N \ge \frac{1}{2}\mathsf{D}(\rho_\Psi,\rho_\Psi)-C\int \rho_\Psi^{\frac{4}{3}}(x)\,dx \tag{25.2.1}$$

with ρ_Ψ defined by (25.1.15).

Remark 25.2.1. Inequality (25.2.1 holds for all (not necessarily antisymmetric) functions Ψ with $\|\Psi\|_{\mathscr{L}^2(\mathbb{R}^{3N})}=1$.

Therefore

$$\begin{aligned}\langle \mathsf{H}_N\Psi,\Psi\rangle \ge \sum_{1\le j\le N}\langle H_{V,x_j}\Psi,\Psi\rangle+\frac{1}{2}\mathsf{D}\bigl(\rho_\Psi,\rho_\Psi\bigr)-C\int\rho_\Psi^{\frac{4}{3}}(x)\,dx=\\ \sum_{1\le j\le N}\langle H_{W,x_j}\Psi,\Psi\rangle+\frac{1}{2}\mathsf{D}\bigl(\rho_\Psi-\rho,\rho_\Psi-\rho\bigr)-\frac{1}{2}\mathsf{D}\bigl(\rho,\rho\bigr)-C\int\rho_\Psi^{\frac{4}{3}}(x)\,dx\end{aligned} \tag{25.2.2}$$

where $\langle\cdot,\cdot\rangle$ means the inner product in $\mathfrak{H}$ and H_W is one-particle Schrödinger operator with the potential

$$W=V-|x|^{-1}*\rho, \tag{25.2.3}$$

where ρ is an arbitrary chosen real-valued non-negative function.

The physical sense of the second term in W is transparent: it is a potential created by a charge $-\rho$. Skipping the positive second term in the right-hand expression of (25.2.2) and believing that the last term is not very important for the ground state function Ψ [4] we see that we need to estimate from below the first term.

Here assumption that Ψ is antisymmetric is crucial. Namely, for general (or symmetric–does not matter) Ψ the best possible estimate is $N\lambda_1$ where λ_1 is the lowest eigenvalue of H_W (we always assume that there is sufficiently many eigenvalues under the bottom of the essential spectrum of H_W) and we

[4] When we derive also an upper estimate for E we will get an upper estimate for this term as a bonus.

cannot apply semiclassical theory. However, for antisymmetric Ψ situation is rather different.

Namely, let $\lambda_1 \le \lambda_2 \le \lambda_3 \le \ldots$ be negative eigenvalues of H_W (on $\mathsf{H} = \mathscr{L}^3(\mathbb{R}^3, \mathbb{C}^q)$. Then the first term in the right-hand expression of (25.2.2) is bounded from below by

$$\sum_{1\le j\le N} \lambda_j = \mathsf{N}_1(H_W - \bar\lambda) + \bar\lambda N \tag{25.2.4}$$

where $\mathsf{N}(B)$, $\mathsf{N}_1(B) = \operatorname{Tr}(B^-)$ are the number and the sum of all the negative eigenvalues of operator B respectively such that $\mathsf{Spec}_{\mathsf{ess}}(B) \subset \mathbb{R}^+$ provided $\bar\lambda = \lambda_N < 0$; the latter assumption is equivalent to

$$\mathsf{N}(H_W) \ge N. \tag{25.2.5}$$

Applying the semiclassical approximation (which needs to be justified!) one gets

$$\mathsf{N}_1(H_W - \bar\lambda) = \mathcal{N}_1(H_W - \bar\lambda) + \mathsf{error}_1 \tag{25.2.6}$$

with

$$\mathcal{N}_1(H_W - \bar\lambda) := -\int P\bigl(W(x) + \bar\lambda\bigr)\, dx \tag{25.2.7}$$

and error_0 *an error in the semiclassical approximation* for $\mathsf{N}_1(H_W - \bar\lambda)$. Therefore the lower estimate for the ground state energy is

$$\mathsf{E} \ge -\int P(W + \bar\lambda)\, dx + \bar\lambda N - \frac{1}{2}\mathsf{D}(\rho, \rho) - \mathsf{error} \tag{25.2.8}$$

where error now includes both an estimate for $\int \rho_\Psi^{\frac{4}{3}}\, dx$ and the semiclassical remainder estimate.

Furthermore, applying a semiclassical approximation for the number $\mathsf{N}(H_W - \bar\lambda)$ of eigenvalues below $\bar\lambda$ (and this number should be approximately N) one gets an equality

$$N = \mathcal{N}(H_W - \bar\lambda) + \mathsf{error}_0 \tag{25.2.9}$$

with

$$\mathcal{N}(H_W - \bar\lambda) := \int P'\bigl(W(x) + \bar\lambda\bigr)\, dx \tag{25.2.10}$$

and error_0 *an error in the semiclassical approximation* for $\mathsf{N}(H_W - \bar\lambda)$.

To get the best possible lower estimate one should pick up ρ delivering maximum to the functional

$$-\int P\bigl(W(x)+\nu\bigr)\,dx + \nu N - \frac{1}{2}\mathsf{D}(\rho,\rho) \tag{25.2.11}$$

($\nu=\bar\lambda$ here) under assumptions $(25.1.21)_{1,2}$ and (25.2.3) as we skip all the errors.

One can see that the optimal choice is the *Thomas-Fermi potential* W^{TF} *and density* ρ^{TF}. The above arguments are very standard in MQT with $\rho=\rho^{\mathsf{TF}}, W=W^{\mathsf{TF}}$ [5] from the very beginning.

On the other hand, let us consider the Euler-Lagrange equation for $\rho=\rho^{\mathsf{TF}}$ under condition $\int\rho\,dx=N$:

$$\tau'(\rho)-W=\nu\quad(\rho>0),\qquad W=V-|x|^{-1}*\rho \tag{25.2.12}$$

with the Lagrange factor ν [6]. Expressing ρ and integrating we get

$$N=\mathcal{N}(H_W-\nu)=\int P'\bigl(W(x)+\nu\bigr)\,dx. \tag{25.2.13}$$

Comparing (25.2.12) and (25.2.13) we get that with some error $\bar\lambda\sim\nu$. Substituting to the first term in (25.2.6) $\bar\lambda=\nu$ and $\nu-W=-\tau_B'(\rho)$ we get the lower estimate $\mathsf{E}\ge\mathcal{E}^{\mathsf{TF}}-\mathsf{error}$.

Remark 25.2.2. (i) Instead of (25.2.6) we will use a better estimate[7];

(ii) To minimize errors we will also recalculate (25.2.4) effectively replacing $\bar\lambda$ by ν:

$$\sum_{1\le j\le N}\lambda_j=\sum_{1\le j\le N}(\lambda_j-\nu)+\nu N\ge\mathsf{N}_1(H_W-\nu)+\nu N. \tag{25.2.14}$$

The advantage is that we even do not mess up with the semiclassical asymptotics for $\mathsf{N}(H_W-\nu)$. Further, one can replace here N by $\int\rho^{\mathsf{TF}}\,dx$: (these quantities fail to be equal only for $N>Z$ i.e. for $\nu=0$).

[5] Or some their close approximations.

[6] Called *chemical potential* and in contrast to $\bar\lambda$ belonging to Thomas-Fermi theory.

[7] With $\mathcal{E}^{\mathsf{TF}}$ replaced by $\mathcal{E}^{\mathsf{TF}}+\mathsf{Scott}+\mathsf{Schwinger}$ and with much smaller error_1 than for a simple semiclassical approximation.

(iii) Recall that we assumed that $\lambda_N < 0$ i.e. (25.2.5) holds. In the opposite case

$$\mathsf{N}(H_W) < N. \tag{25.2.15}$$

we estimate the first term in the right-hand expression of (25.2.2) from below by $\mathsf{N}_1(H_W)$ i.e. we will get the same formula but with $\nu = 0$.

25.2.2 Upper Estimate

To get the upper estimate one takes a test function $\Psi(x_1, \dots, x_N)$ which is not a ground state here but an antisymmetrization with respect to $(x_1, \dots, x_N)$ of the product $\phi_1(x_1)\cdots\phi_N(x_N)$ where $\phi_1, \dots, \phi_N$ are orthonormal eigenfunctions of H_W corresponding to eigenvalues $\lambda_1, \dots, \lambda_N$, provided $\lambda_N < 0$. Namely this function minimizes the first term in the right-hand expression of (25.2.2).

One can write

$$\Psi = \frac{1}{N!}\det\bigl(\phi_i(x_j)\bigr)_{i,j=1,\dots,N} \tag{25.2.16}$$

and it is called the *Slater determinant*. Obviously, $\|\Psi\| = 1$ and

$$\rho_\Psi(x) = \operatorname{tr} e_N(x,x) \tag{25.2.17}$$

where

$$e_N(x,y) = \sum_{1\le j\le N} \phi_j(x)\phi_j^\dagger(y) \tag{25.2.18}$$

is the Schwartz kernel of the projector to the subspace spanned on $\{\phi_j\}_{1\le j\le N}$.

Remark 25.2.3. If $q \ge 2$ then $\phi_j = \phi_j(x,\varsigma)$ and $\Psi(x_1,\varsigma_1;\dots;x_N,\varsigma_N)$ is an antisymmetrization with respect to $(x_1,\varsigma_1;\dots;x_N,\varsigma_N)$ of the product $\phi_1(x_1,\varsigma_1)\cdots\phi_N(x_N,\varsigma_N)$.

Easy calculations show that

$$\begin{aligned}\langle \mathsf{H}\Psi,\Psi\rangle = \sum_{1\le j\le N}\lambda_j + \frac{1}{2}\mathsf{D}(\rho_\Psi-\rho,\rho_\Psi-\rho)\\ -\frac{1}{2}\mathsf{D}(\rho,\rho) - \frac{1}{2}\iint |x-y|^{-1}\operatorname{tr} e_N^\dagger(x,y)e_N(x,y)\,dxdy.\end{aligned} \tag{25.2.19}$$

The first term in the right-hand expression again is equal to the middle expression in (25.2.4) which does not exceed

$$\mathsf{N}_1(H_W-\nu)+\nu N+|\lambda_N-\nu|\cdot|\mathsf{N}(H_W-\nu)-N|. \tag{25.2.20}$$

Really, we need to consider (non-zero) terms which do not cancel in

$$\sum_{j\le N}(\lambda_j-\nu)-\sum_{\lambda_j<\nu}(\lambda_j-\nu) \tag{25.2.21}$$

and their absolute value does not exceed $|\lambda_N-\nu|$ while their number does not exceed $|\mathsf{N}(H_W-\nu)-N|$.

Again, discounting all the errors and considering semiclassical approximation (including $\rho_\Psi(x)\sim P'\bigl(W(x)+\nu\bigr)$) we arrive to a functional

$$-\int P\bigl(W(x)+\nu\bigr)\,dx+\nu N-\frac{1}{2}\mathsf{D}(\rho,\rho)+\\ \frac{1}{2}\mathsf{D}(P'(W+\nu)-\rho,P'(W+\nu)-\rho) \tag{25.2.22}$$

which needs to be minimized under assumptions $(25.1.21)_{1,2}$ and (25.2.3). This functional differs from (25.2.11) which was minimized by the last term. One can prove that (25.2.22) minimizes as $\rho=\rho^{\mathsf{TF}}$, $W=W^{\mathsf{TF}}$ and ν is a chemical potential. So again we may pick them (or their appropriate approximations) up from the very beginning.

Therefore in addition to a semiclassical error_1 [7] of the previous subsection we need to consider also semiclassical errors

$$\mathsf{D}\bigl(\operatorname{tr} e(x,x,\nu)-P'(W+\nu),\operatorname{tr} e(x,x,\nu)-P'(W+\nu)\bigr), \tag{25.2.23}$$

$$\mathsf{D}\bigl(e(x,x,\nu)-e_N(x,x),e(x,x,\nu)-e_N(x,x)\bigr) \tag{25.2.24}$$

where $e(x,y,\nu)$ is the Schwartz kernel of the spectral projector $\uptheta(\tau-H_W)$ of H_W,

$$N(H_W-\nu)-\int P'(W+\nu)\,dx \tag{25.2.25}$$

and

$$\lambda_N-\nu. \tag{25.2.26}$$

Remark 25.2.4. (i) Recall that we assumed that $\lambda_N < 0$ i.e. (25.2.5) holds. In the opposite case (25.2.15) selecting appropriate $\phi_j(x)$ with $j = \mathsf{N}(H_W) + 1, \dots, N$ we with arbitrarily small error estimate the first term in the right-hand expression of (25.2.2) from above by $\mathsf{N}_1(H_W)$ as i.e. we will get the same formula but with $\nu = 0$ and we also will need to estimate (25.2.23) with $\nu = 0$.

(ii) To make this case compatible with the case (25.2.5) we will need to estimate $|\nu|$ (and $|N - Z|$) under assumption (25.2.15); we will also compare $\mathcal{E}^{\mathsf{TF}}$ calculated for such ν (or, equivalently, N as they are connected) and $\nu = 0$ (and $N = Z$).

(iii) Sure ρ^{TF} and W^{TF} depend on ν (or N) but we will prove that for $N - Z$ relatively small we can do all calculations as $\nu = 0$ (and $N = Z$).

(iv) If we are interested in the estimate for $\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}}, \rho_\Psi - \rho^{\mathsf{TF}})$ where Ψ is the ground state, we do not need to calculate a semiclassical error in $\mathsf{N}_1(H_W - \nu)$. In fact, we can simply stick with $\mathsf{N}_1(H_W - \bar{\lambda})$ with $\bar{\lambda} = \lambda_N$ under assumption (25.2.5) and $\bar{\lambda} = 0$ otherwise. As a result in certain cases our estimate for $\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}}, \rho_\Psi - \rho^{\mathsf{TF}})$ will be better than the error in an approximation for E and we need the former rather than the latter for the results of the second half of this Chapter. Especially significant the difference will be when we introduce magnetic field.

25.2.3 Remarks and Dirac Correction

Now almost everything is in framework of the theory we developed; the only missing is an estimate

$$\int \rho_\Psi^{\frac{4}{3}}\, dx \le CZ^{\frac{5}{3}} \tag{25.2.27}$$

for a reasonable candidate Ψ to the ground state; one can find it in E. Lieb's *Selecta*[3)].

However if we want a more sharp asymptotics with Dirac–Schwinger terms, we need a remainder estimate $o(Z^{\frac{5}{3}})$ or better; luckily there is improved electrostatic inequality due to Theorem 1, G. Graf and J. P. Solovej [1] (see also V. Bach [1]).

Theorem 25.2.5. *Let $N \ge \epsilon Z$. Then for the ground state Ψ*

$$\mathsf{E}_{\mathsf{HF}} \ge \mathsf{E} \ge \mathsf{E}_{\mathsf{HF}} - CZ^{\frac{5}{3}-\delta} \tag{25.2.28}$$

and

$$\mathsf{E} \ge \mathsf{E}_{\mathsf{DS}} - CZ^{\frac{5}{3}-\delta} \tag{25.2.29}$$

with some exponent $\delta > 0$ where

$$\mathsf{E}_{\mathsf{HF}} := \inf_{\Psi} E_{\mathsf{HF}}(\Psi), \tag{25.2.30}$$

where in (25.2.30) Ψ *runs through Slater determinants*[8] *and*

$$E_{\mathsf{HF}}(\Psi) := \sum_{1\le j\le N} \langle H_{V,x_j}\Psi, \Psi\rangle + \frac{1}{2}\mathsf{D}\bigl(\rho_\Psi, \rho_\Psi\bigr) - \frac{1}{2}\iint |x-y|^{-1}\operatorname{tr} e_N^\dagger(x,y)e_N(x,y)\,dxdy, \tag{25.2.31}$$

$$E_{\mathsf{DS}} := \sum_{j:1\le j\le N;\lambda_j<0} \lambda_j - \frac{1}{2}\mathsf{D}(\rho^{\mathsf{TF}}, \rho^{\mathsf{TF}}) - \kappa_{\mathsf{Dirac}}\int \rho^{\mathsf{TF},\frac{4}{3}}\,dx, \tag{25.2.32}$$

$\kappa_{\mathsf{Dirac}} = (2\pi)^{-3}qc_{\mathsf{TF}}^2$, $c_{\mathsf{TF}} = (6\pi^2/q^2)^{\frac{2}{3}}$ *is a Dirac constant.*

Here (25.2.28)–(25.2.31) are (1.15), (1.16), (1.8), (1.6) respectively and (25.2.32) is a combination of (1.12) and (25.3.30) of this paper[9]. Actually we need only (25.2.29) and (25.2.32).

As we are going to prove that the last terms in (25.2.31) and (25.2.19) coincide modulo $O(Z^{\frac{5}{3}-\delta})$ we made a necessary step completely.

25.3 Thomas-Fermi Theory

Thomas-Fermi theory is well-developed in the no-magnetic-field case. We cannot suggest any better reading than E. Lieb's *Selecta*[3].

In the Thomas-Fermi theory N is a real nonnegative number (not necessarily an integer).

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[8] Albeit not necessarily of eigenfunctions of H_W.

[9] We do not have a coefficient $\frac{1}{2}$ in the definition of $\mathsf{D}(.,.)$ but G. Graf and J. P. Solovej [1] have.

25.3.1 Existence

Let us recall that in order to get the best lower estimate (neglecting semi-classical errors) one needs to maximize

$$\Phi_*(W+\nu) := -\int P(W+\nu)\,dx - \frac{1}{8\pi}\|\nabla(W-V)\|^2 \tag{25.3.1}$$

given by (25.2.11) where we used equalities

$$\mathsf{D}(\rho,\rho) = -(\rho, W-V) = \frac{1}{4\pi}\|\nabla(W-V)\|^2, \tag{25.3.2}$$

$$\rho := \frac{1}{4\pi}\Delta(W-V), \tag{25.3.3}$$

$\|.\|$ means $\mathscr{L}^2$-norm and $W\to 0$ as $|x|\to\infty$.

On the other hand, to get the best possible upper estimate (neglecting semiclassical errors) one needs to minimize

$$\Phi^*(\rho',\nu) := \int \bigl(\tau(\rho') - V\rho'\bigr)\,dx + \frac{1}{2}\mathsf{D}(\rho',\rho') - \nu\int \rho'\,dx \tag{25.3.4}$$

where

$$\rho' := P'(W+\nu) \tag{25.3.5}$$

and $\tau(\rho)$ the Legendre transformation (25.1.18) of P. Recall that according to (25.1.19)

$$P(w) = \frac{q}{15\pi^2}w_+^{\frac{5}{2}}, \qquad P'(w) = \frac{q}{6\pi^2}w_+^{\frac{3}{2}} \tag*{(25.3.6)$_{1,2}$}$$

and therefore

$$\tau(\rho) = \frac{3}{5}\bigl(6\pi^2 q^{-1}\bigr)^{\frac{2}{3}}\rho^{\frac{5}{3}}. \tag{25.3.7}$$

Proposition 25.3.1. *In our assumptions for any fixed* $\nu\le 0$

(i) $\Phi_*(W+\nu)$ *is a strictly concave functional.*

(ii) $\Phi^*(\rho)$ *is a strictly convex functional.*

(iii) $\Phi_*(W+\nu)\le \Phi^*(\rho,\nu)$ *for any* $\rho\ge 0$ *and* W.

(iv) These extremal problems have a common solution W *and* ρ *and*

$$\rho = \frac{1}{4\pi}\Delta(W-V) = P'(W+\nu), \tag{25.3.8}$$

$$W = o(1) \qquad \textit{as}\ \ |x|\to\infty. \tag{25.3.9}$$

(v) On the other hand, solution of (25.3.8)–(25.3.9) *is the solution of the both extremal problems.*

(vi) Neither of these problem has a solution for $\nu > 0$.

(vii) Function

$$\mathcal{N}(\nu) = \int P'(W+\nu)\,dx \tag{25.3.10}$$

is continuous and monotone increasing at $(-\infty, 0]$ *with* $\mathcal{N}(\nu) \to 0$ *as* $\nu \to -\infty$ *and* $\mathcal{N}(0) = Z$.

(viii) For ν *and* N *linked by* $N = \mathcal{N}(\nu)$ *solutions of the problem above coincide with* $\rho^{\mathsf{TF}}, W^{\mathsf{TF}}$ *of the problem* (25.1.20) *and one can skip condition* $(25.1.20)_2$ *for* $N \geq Z$ *and*

$$\mathcal{E}^{\mathsf{TF}} = \Phi(W^{\mathsf{TF}} + \nu) + \nu N = \Phi^*(\rho^{\mathsf{TF}}, \nu) + \nu N. \tag{25.3.11}$$

Proof. The proof of Statements (i) and (ii) is obvious; therefore both problems have unique solutions. Comparing Euler-Lagrange equations we get that these solutions coincide which yields Statements (iv) and (iii).

Proof of Statements (v)–(viii) is also rather obvious. □

Proposition 25.3.2. *For arbitrary* W *the following estimates hold with absolute constants* $\epsilon_0 > 0$ *and* C_0*:*

$$\epsilon_0 \mathsf{D}(\rho - \rho^{\mathsf{TF}}, \rho - \rho^{\mathsf{TF}}) \leq \Phi_*(W^{\mathsf{TF}} + \nu) - \Phi_*(W+\nu) \leq C_0 \mathsf{D}(\rho - \rho', \rho - \rho') \tag{25.3.12}$$

and

$$\epsilon_0 \mathsf{D}(\rho' - \rho^{\mathsf{TF}}, \rho' - \rho^{\mathsf{TF}}) \leq \Phi^*(\rho, \nu) - \Phi^*(\rho^{\mathsf{TF}}, \nu) \leq C_0 \mathsf{D}(\rho - \rho', \rho - \rho') \tag{25.3.13}$$

with $\rho = \frac{1}{4\pi}\Delta(W - V)$, $\rho' = P'(W+\nu)$.

Proof. This proof is rather obvious as well. □

25.3.2 Properties

Proposition 25.3.3. *The solution of the Thomas-Fermi problem has following scaling properties*

$$W^{\mathsf{TF}}(x;\ \underline{Z};\ \underline{y};\ N;\ q) = q^{\frac{2}{3}} N^{\frac{4}{3}} W^{\mathsf{TF}}(q^{\frac{2}{3}} Z^{\frac{1}{3}} x;\ N^{-1}\underline{Z};\ q^{\frac{2}{3}} N^{\frac{1}{3}}\underline{y};\ 1;\ 1), \tag{25.3.14}$$

$$\rho^{\mathsf{TF}}(x;\ \underline{Z};\ \underline{y};\ N;\ q) = N^2 q^2 \rho^{\mathsf{TF}}(q^{\frac{2}{3}} Z^{\frac{1}{3}} x;\ N^{-1}\underline{Z};\ q^{\frac{2}{3}} N^{\frac{1}{3}}\underline{y};\ 1;\ 1), \tag{25.3.15}$$

$$\mathcal{E}^{\mathsf{TF}}(\underline{Z};\ \underline{y};\ N;\ q) = q^{\frac{2}{3}} N^{\frac{7}{3}} \mathcal{E}^{\mathsf{TF}}(N^{-1}\underline{Z};\ q^{\frac{2}{3}} N^{\frac{1}{3}}\underline{y};\ 1;\ 1), \tag{25.3.16}$$

$$\nu^{\mathsf{TF}}(\underline{Z};\ \underline{y};\ N;\ q) = q^{\frac{2}{3}} N^{\frac{4}{3}} \nu^{\mathsf{TF}}(N^{-1}\underline{Z};\ q^{\frac{2}{3}} N^{\frac{1}{3}}\underline{y};\ 1;\ 1) \tag{25.3.17}$$

where $\nu^{\mathsf{TF}} = \nu$ *is the chemical potential; recall that* $\underline{Z} = (Z_1, \dots, Z_M)$ *and* $\underline{\mathsf{y}} = (\mathsf{y}_1, \dots, \mathsf{y}_M)$ *are arrays and parameter* q *also enters into Thomas-Fermi theory.*

Proof. Proof is trivial by scaling. □

Since we can exclude q by scaling, we do not indicate dependence on it anymore. The following properties of Thomas-Fermi potential and density in the case of the single atom ($M = 1$) are well-known:

Proposition 25.3.4. *Let* $M = 1$*. Then the solution of the Thomas-Fermi problem has the following properties:*

(i) $W^{\mathsf{TF}}(x; Z_m, \mathsf{y}_m; N)$ *and* $\rho^{\mathsf{TF}}(x; Z_m, \mathsf{y}_m; N)$ *are spherically symmetric (with respect to* y_m*) and are non-increasing convex functions of* $|x - \mathsf{y}_m|$*.*

(ii) If $N = Z_m$*, then*

$$W^{\mathsf{TF}} \asymp \min\bigl(Z_m|x - \mathsf{y}_m|^{-1}, |x - \mathsf{y}_m|^{-4}\bigr), \tag{25.3.18}$$

$$\rho^{\mathsf{TF}} \asymp \min\bigl(Z_m^{\frac{3}{2}}|x - \mathsf{y}_m|^{-\frac{3}{2}}, |x - \mathsf{y}_m|^{-6}\bigr) \tag{25.3.19}$$

with the threshold at $|x - \mathsf{y}_m| \asymp r_m^* = Z_m^{-\frac{1}{3}}$ *when* $W^{\mathsf{TF}} \asymp Z_m^{\frac{4}{3}}$ *and* $\rho^{\mathsf{TF}} \asymp Z_m^2$*.*

(iii) If $\epsilon Z_m \le N < Z_m$*, then*

$$-\nu \asymp |Z_m - N|^{\frac{4}{3}} \tag{25.3.20}$$

and (25.3.18) *holds as* $|x - \mathsf{y}_m| \le \bar{r}_m$ *where*

$$\bar{r}_m = -\nu^{-1}|Z_m - N|^{-1} \asymp |Z_m - N|^{-\frac{1}{3}} \tag{25.3.21}$$

for atoms denotes the exact radius of the support of ρ^{TF} *(see Statement (iv).*

(iv) On the other hand,

$$W^{\mathsf{TF}} = (Z_m - N)|x - y_m|^{-1} \qquad \text{as} \quad |x - y_m| \geq \bar{r}_m \tag{25.3.22}$$

and $\rho^{\mathsf{TF}} = 0$ *as* $|x - y_m| \geq \bar{r}_m$*;*

(v) Meanwhile, $W^{\mathsf{TF}} \asymp -\nu$ *and* $\rho^{\mathsf{TF}} = O\bigl(|Z_m - N|^2\bigr)$ *as* $|x - y_m| \asymp \bar{r}_m$*.*

(vi) Finally,

$$-\langle x - y_m, \nabla W\rangle \asymp W. \tag{25.3.23}$$

Consider now the molecular case ($M \geq 2$):

Proposition 25.3.5. *(i) Let* $M \geq 2$*. Then*

$$\nu \asymp |Z - N|^{\frac{4}{3}} \tag{25.3.24}$$

and

$$\sum_m \epsilon W_m^{\mathsf{TF}}(c(x - y_m)) \leq W^{\mathsf{TF}} \leq c \sum_m W_m^{\mathsf{TF}}(\epsilon(x - y_m)) \tag{25.3.25}$$

where $Z = Z_1 + \ldots + Z_M$ *and* W_m^{TF} *denotes an atomic Thomas-Fermi potential with the charge* Z_m *located at* 0 *and the same chemical potential* ν*. Here* ϵ *and* c *depend only on* M*.*

(ii) In particular, if $N < Z$ *and* $|x - y_m| \geq c\bar{r}_m$ *for all* $m = 1, \ldots, M$*, then*

$$W^{\mathsf{TF}}(x) \asymp \sum_m |Z - N||x - y_m|^{-1} \tag{25.3.26}$$

and

$$\rho^{\mathsf{TF}}(x) = 0. \tag{25.3.27}$$

Proof. Proof is due to the comparison arguments of E. Lieb, J. P. Solovej and J. Yngvason [1,3]. □

Proposition 25.3.6. *(i) Let* $N \leq Z$ *and*

$$\ell(x) = \frac{1}{2} \min_m |x - y_m|, \tag{25.3.28}$$

$$\zeta(x) = \bigl(W^{\mathsf{TF}}(x)\bigr)^{\frac{1}{2}}. \tag{25.3.29}$$

Then

$$\zeta(x) \le \bar{\zeta}(x) = C\begin{cases} Z^{\frac{1}{2}}\ell(x)^{-\frac{1}{2}} & as\ \ \ell(x)\le Z^{-\frac{1}{3}},\\ \ell(x)^{-2} & as\ \ Z^{-\frac{1}{3}}\le \ell(x)\le |Z-N|^{-\frac{1}{3}},\\ |Z-N|^{\frac{1}{2}}\ell(x)^{-\frac{1}{2}} & as\ \ \ell(x)\ge |Z-N|^{-\frac{1}{3}};\end{cases} \tag{25.3.30}$$

$\zeta(x)$ *and* $\bar{\zeta}(x)$ *are both* ℓ*-admissible and*

$$\bigl|D^\alpha W^{\mathsf{TF}}(x)\bigr| \le C_\alpha \zeta(x)^2\,\ell(x)^{-|\alpha|}\qquad \forall \alpha: |\alpha|\le 3, \tag{25.3.31}$$

and

$$|D^\alpha W^{\mathsf{TF}}(x) - D^\alpha W^{\mathsf{TF}}(y)| \le C_3\zeta(x)^2\ell(x)^{-\frac{7}{2}}|x-y|^{\frac{1}{2}}\qquad \forall x,y: |x-y|\le \epsilon\ell(x) \tag{25.3.32}$$

(ii) Unless $\zeta(x)\asymp(-\nu)^{\frac{1}{2}}$ *estimates* (25.3.32) *hold for all* α*.*

Proof. This proof is rather obvious corollary of the Euler-Lagrange equation. □

Remark 25.3.7. Let

$$Z_m \asymp N\qquad \forall m. \tag{25.3.33}$$

Then $\zeta(x)\asymp\bar{\zeta}(x)$.

Theorem 25.3.8 [10]**.** *Consider* $\mathcal{E}^{\mathsf{TF}}$ *and*

$$\widehat{\mathcal{E}}^{\mathsf{TF}} := \mathcal{E}^{\mathsf{TF}} + U, \tag{25.3.34}$$

$$U = U(Z_1,\dots,Z_M;\mathsf{y}_1,\dots,\mathsf{y}_M) = \sum_{1\le m<m'\le M}\frac{Z_mZ_{m'}}{|\mathsf{y}_m-\mathsf{y}_{m'}|}. \tag{25.3.35}$$

Select a nucleus y_m *and a unit vector* n *such that*

$$\langle \mathsf{y}_k-\mathsf{y}_m,\mathsf{n}\rangle\le 0\qquad \forall k \tag{25.3.36}$$

and plug $\mathsf{y}_m+\alpha\mathsf{n}$ *instead of* y_m *into* $\mathcal{E}^{\mathsf{TF}}$ *and into* $\widehat{\mathcal{E}}^{\mathsf{TF}}$ [11]*. Then*

[10] Theorem 1 of R. Benguria [1]; we combine two last statements in (iii).
[11] So all other nuclei are confined in half-space and y_m moves away outside.

(i) $\widehat{\mathcal{E}}^{\mathsf{TF}}_\alpha$ *is a non-increasing function of* $\alpha \ge 0$*;*

(ii) $\mathcal{E}^{\mathsf{TF}}_\alpha$ *is a non-increasing function of* $\alpha \ge 0$*;*

(iii) For fixed $\alpha > 0$ *both* $\widehat{\mathcal{E}}^{\mathsf{TF}}_\alpha - \widehat{\mathcal{E}}^{\mathsf{TF}}_0$ *and* $\mathcal{E}^{\mathsf{TF}}_\alpha - \mathcal{E}^{\mathsf{TF}}_0$ *are non-decreasing functions of* N*.*

Equality

$$\nu = \frac{\partial \mathcal{E}^{\mathsf{TF}}}{\partial N} \tag{25.3.37}$$

implies that (iii) is equivalent to

$$\nu_\alpha \ge \nu_0. \tag{25.3.38}$$

Theorem 25.3.9 [12]**.** *(i) For fixed* $Z_1, \dots, Z_M; \mathsf{y}_1, \dots, \mathsf{y}_M$ *and* $N = Z$

$$\lambda^7 \widehat{\mathcal{E}}^{\mathsf{TF}}(\underline{Z}; \lambda\underline{\mathsf{y}}; N) = \widehat{\mathcal{E}}^{\mathsf{TF}}(\lambda^3\underline{Z}; \underline{\mathsf{y}}; \lambda^3 N) \tag{25.3.39}$$

is positive non-decreasing function of $\lambda > 0$ *and has a finite limit as* $\lambda \to +\infty$*.*

(ii) This limit does not depend on $Z_1, \dots, Z_M$*.*

Remark 25.3.10. One can observe easily that the same scaling property without assumption $N = Z$ holds for $\mathcal{E}^{\mathsf{TF}}$ and U as well.

These two theorems and remark imply immediately

Proposition 25.3.11. *Let assumption* (25.3.33) *be fulfilled. Then*

$$\widehat{\mathcal{E}}^{\mathsf{TF}}(\underline{Z}; \underline{\mathsf{y}}; N) - \min_{\substack{N_1,\dots,N_M:\\ N_1+\dots N_M = N}} \sum_{1\le m\le M} \mathcal{E}^{\mathsf{TF}}(Z_m; N_m) \ge \epsilon \min(a^{-7}, Z^{\frac{7}{3}}) \tag{25.3.40}$$

where

$$a = \frac{1}{2}\min_{m<m'} |\mathsf{y}_m - \mathsf{y}_{m'}|. \tag{25.3.41}$$

Proof. In virtue of theorem 25.3.8(i) it suffices to prove proposition for $M = 2$ (all other nuclei could be pulled to infinity), and in virtue of theorem 25.3.8(iii) it suffices to prove proposition for $Z = N$.

Then the proof is due to theorem 25.3.9(i) and (25.3.33), which provides uniformity. □

[12] (1.8)–(1.9) of H. Brezis and E. Lieb [1].

Remark 25.3.12. In virtue of (25.3.37) the minimum (with respect to $N_1, \dots, N_M$) in the sum in the right hand expression is reached when $\nu_j = \nu_k$ for all j, k. The same is true for a system of isolated molecules.

Proposition 25.3.13. *Let $\mathcal{Q}$ denote Thomas-Fermi excess energy which is the left-hand expression of* (25.3.40). *Then*

$$\mathsf{D}(\rho^{\mathsf{TF}} - \bar{\rho}^{\mathsf{TF}}, \rho^{\mathsf{TF}} - \bar{\rho}^{\mathsf{TF}}) \le C\mathcal{Q}, \qquad \bar{\rho}^{\mathsf{TF}} := \sum_{1\le m\le M} \rho_m^{\mathsf{TF}}. \tag{25.3.42}$$

Proof. We follow "non-binding" proof due to Baxter (see E. Lieb *Selecta*[3)]).

According to Baxter's lemma there exist g, $0 \le g \le \rho^{\mathsf{TF}}$ and $h = \rho^{\mathsf{TF}} - g$ such that $g * |x|^{-1} = V_1$ a.e. when $h > 0$ and $g * |x|^{-1} \le V_1$ a.e. when $h = 0$. Here $V_m = Z_m|x - \mathsf{y}_m|^{-1}$.

Let $\alpha = \int g\,dx$, $\beta = \int h\,dx$ and let $\mathcal{E}_1^{\mathsf{TF}}$, $\mathcal{E}_{(1)}^{\mathsf{TF}}$ be Thomas-Fermi energies for the first atom and for the rest of molecule respectively and ρ_1^{TF}, $\rho_{(1)}^{\mathsf{TF}}$ be corresponding Thomas-Fermi densities. Then

$$\begin{gathered}\min_{N_1+N'\le N}\Bigl(\mathcal{E}_1^{\mathsf{TF}}(N_1) + \mathcal{E}_{(1)}^{\mathsf{TF}}(N')\Bigr) \le \mathcal{E}_1(\alpha) + \mathcal{E}_{(1)}(\beta) \le \\ \mathcal{E}_1(g) + \mathcal{E}_{(1)}(h) - \epsilon\mathsf{D}(g - \rho_1^{\mathsf{TF}}, g - \rho_1^{\mathsf{TF}}) - \epsilon\mathsf{D}(h - \rho_{(1)}^{\mathsf{TF}}, h - \rho_{(1)}^{\mathsf{TF}}) \le \\ \mathcal{E}(g+h) + \int h(V_1 - g * |x|^{-1})\,dx - \int (V_1 - |g * |x|^{-1})\,d\upmu_{(1)} \\ - \epsilon\mathsf{D}(g - \rho_1^{\mathsf{TF}}, g - \rho_1^{\mathsf{TF}}) - \epsilon\mathsf{D}(h - \rho_{(1)}^{\mathsf{TF}}, h - \rho_{(1)}^{\mathsf{TF}})\end{gathered} \tag{25.3.43}$$

where $\upmu_1$ and $\upmu_{(1)}$ are measures with the densities respectively $Z_1\delta(x - \mathsf{y}_1)$ and $\sum_{2\le m\le M} Z_m\delta(x - \mathsf{y}_m)$ and we used the superadditivity of $\tau(\rho) = \rho^{\frac{5}{3}}$. The last expression does not exceed

$$\mathcal{E}^{\mathsf{TF}} - \epsilon\mathsf{D}(g - \rho_1^{\mathsf{TF}}, g - \rho_1^{\mathsf{TF}}) - \epsilon\mathsf{D}(h - \rho_{(1)}^{\mathsf{TF}}, h - \rho_{(1)}^{\mathsf{TF}}). \tag{25.3.44}$$

Using induction with respect to M we arrive to

$$\begin{gathered}\mathsf{D}(\rho^{\mathsf{TF}} - \rho_1^{\mathsf{TF}} - \rho_{(1)}^{\mathsf{TF}}, \rho^{\mathsf{TF}} - \rho_1^{\mathsf{TF}} - \rho_{(1)}^{\mathsf{TF}}) \le \\ 2\mathsf{D}(g - \rho_1^{\mathsf{TF}}, g - \rho_1^{\mathsf{TF}}) + 2\mathsf{D}(h - \rho_{(1)}^{\mathsf{TF}}, h - \rho_{(1)}^{\mathsf{TF}}) \le C\mathcal{Q}\end{gathered} \tag{25.3.45}$$

and finally to (25.3.42). ∎

Problem 25.3.14. Find the stronger lower bound in (25.3.40) as $N < Z$. Would be the left-hand expression $\asymp \min(a^{-7} + |Z - N|^2 a^{-1}, Z^{\frac{7}{3}})$?

25.4 Application of Semiclassical Methods

25.4.1 Asymptotics of the Trace

In this subsection we calculate asymptotics of $\mathsf{Tr}((H_W-\nu)^-)$. Here we need to consider both inner and outer zones.

An *inner zone* (near nucleus y_m) is a ball where $V_j=Z_m|x-\mathsf{y}_m|^{-1}$ dominates $W-V_m$. For a single nucleus ($M=1$) it is defined by

$$|x-\mathsf{y}_m|\le \epsilon Z_m^{-\frac{1}{3}} \tag{25.4.1}$$

but in the case $M\ge 2$ there are another restrictions

$$|x-\mathsf{y}_m|\le \epsilon \min_{m'\ne m}\Bigl(Z_m(Z_m+Z_{m'})^{-1}|\mathsf{y}_m-\mathsf{y}_{m'}|\Bigr) \tag{25.4.2}$$

and

$$|x-\mathsf{y}_m|\le Z_m\nu^{-1} \tag{25.4.3}$$

but we shrink this zone to

$$|x-\mathsf{y}_m|\le r_m\coloneqq \epsilon \min\bigl(Z_mZ^{-1}a, Z_m^{-\frac{1}{3}}\bigr). \tag{25.4.4}$$

Let us consider contribution of the zone $\mathcal{X}_m$ described by (25.4.4) to $\mathsf{N}_1(H_W-\nu)=\mathsf{Tr}((H_W-\nu)^-)$, both into the principal part of asymptotics and the remainder. Let ψ_m be a partition element concentrated in $\mathcal{X}_m$ and equal to 1 in $\{x\colon |x-\mathsf{y}_m|\le \frac{1}{2}r_m\}$. Then, according to Theorem 12.6.8,

$$\mathsf{Tr}\bigl((H_W-\nu)^-\psi_m\bigr)=\int \mathsf{Weyl}_1(x)\psi_m(x)\,dx+\mathsf{Scott}_m+O(R_m) \tag{25.4.5}$$

where $\mathsf{Weyl}_1(x)$ and Scott_m are calculated for the case $q=1$ and then multiplied by q [13]:

$$\mathsf{Weyl}_1(x)\coloneqq -\frac{q}{15\pi^2}\bigl(W(x)+\nu\bigr)_+^{\frac{5}{2}} \tag{25.4.6}$$

while R_m is $C\zeta^2(\zeta\ell)=C\zeta^3\ell$ calculated on its border i.e.

$$R_m=CZ_m^{\frac{5}{3}}+CZ_m^{\frac{3}{2}}r_m^{-\frac{1}{2}}\le CZ^{\frac{5}{3}}+CZ^{\frac{3}{2}}a^{-\frac{1}{2}}. \tag{25.4.7}$$

Really, one needs just to rescale $x\mapsto (x-\mathsf{y}_m)r_m^{-1}$ and $\tau\mapsto \tau Z_m^{-1}r_m$ and introduce a semiclassical parameter $\hbar=Z_m^{\frac{1}{2}}r_m^{\frac{1}{2}}$.

[13] As operator $H_w-\nu$ is nothing but q copies of $\Delta-(W+\nu)$.

Remark 25.4.1. (i) Clearly, these arguments work only if $r_m \ge Z_m^{-1}$ (i.e. $Z_m^2 \ge a^{-1}Z$).

(ii) On the other hand, if $Z_m^2 \ge a^{-1}Z$ but $a \ge Z^{-1}$ we define $r_m = a^{\frac{1}{2}}Z^{-\frac{1}{2}}$ and we do not include Scott_m [14] into the principal expression; moreover, in this case we include $\mathcal{X}_m$ into a singular zone and use variational methods to estimate its contribution into the principal part of asymptotics; it will not exceed $CZa^{-1} \le CZ^{\frac{3}{2}}a^{-\frac{1}{2}}$.

(iii) Furthermore, if $a \le Z^{-1}$, we set $r_m = Z^{-1}$ and we do not include any Scott_m [14] into the principal part of asymptotics and include all $\mathcal{X}_m$ into singular zones; using variational methods we estimate their contributions into the principal part of asymptotics by CZ^2.

Therefore we conclude that

(25.4.8) The total contribution of all inner zones into remainder does not exceed the right-hand expression of (25.4.7) as $a \ge Z^{-1}$ and CZ^2 as $a \le Z^{-1}$.

Let us consider contributions of the *outer zone* $\mathcal{X}_0$ which is complimentary to the union of all inner zones. Then

$$\operatorname{Tr}\bigl((H_W - \nu)^- \psi_0\bigr) = \int \mathsf{Weyl}_1(x)\psi_0(x)\, dx + O(R_0) \tag{25.4.9}$$

with $\mathsf{Weyl}_1(x)$ defined by (25.4.6) where

$$R_0 = \int_{\mathcal{X}_0} C\bar{\zeta}(x)^3 \ell^{-2}\, dx \tag{25.4.10}$$

and

$$\bar{\zeta} = \begin{cases} Z^{\frac{1}{2}}\ell^{-\frac{1}{2}} & \text{as } \ \ell \le Z^{-\frac{1}{3}}, \\ \ell^{-2} & \text{as } \ \ell \ge Z^{-\frac{1}{3}}. \end{cases} \tag{25.4.11}$$

We justify (25.4.9)–(25.4.11) a bit later by an appropriate partition of unity. One can see easily that the contribution of the zone $\{x\colon \ell(x) \le Z^{-\frac{1}{3}}\}$ into expression (25.4.10) does not exceed the same expression as in (25.4.8) and that the contribution of the zone $\{x\colon \ell(x) \ge Z^{-\frac{1}{3}}\}$ into (25.4.10) does not exceed $CZ^{\frac{5}{3}}$. Then we arrive to

[14] However it will be less than the remainder estimate, so we can include it into the principal part of asymptotics anyway.

Theorem 25.4.2. *Let $W = W^{\mathsf{TF}}$, $N \asymp Z$, $W = W^{\mathsf{TF}}$. Then*

$$\mathsf{Tr}\bigl((H_W-\nu)^-\bigr) = \int \mathsf{Weyl}_1(x)\,dx + \sum_{1\le m\le M} \mathsf{Scott}_m + O(R), \tag{25.4.12}$$

with

$$R := \begin{cases} CZ^{\frac{5}{3}} + CZ^{\frac{3}{2}}a^{-\frac{1}{2}} & \text{as}\quad a\ge Z^{-1},\\ CZ^2 & \text{as}\quad a\le Z^{-1}.\end{cases} \tag{25.4.13}$$

Proof. (i) Consider $\nu=0$ first. Then we just apply ℓ-admissible partition of unity. Sure, $\zeta\ell\le 1$ as $\ell\ge 1$ but we can deal with it either by taking $\zeta=\ell^{-1}$ here or considering it as a singular zone and applying here variational estimate as well.

(ii) Variational estimate works for $\nu<0$ as well; furthermore, zone $\{x\colon W(x)\le (1-\epsilon)\nu, \ell\ge |\nu|^{-\frac{1}{2}}\}$ is classically forbidden.

(iii) However as $\nu\le -c$ we have a little problem as W^{TF} is not very smooth, it is only $\mathscr{C}^{\frac{7}{2}}$ as $W\asymp -\nu$. The best[15)] way to deal with it is to take $\varepsilon\ell$-mollification with $\varepsilon=\hbar^{1-\delta}$, $\hbar=(\zeta\ell)^{-1}$, use rough microlocal analysis of Section 4.6 and the bracketing; it will bring an approximation error not exceeding $C\varepsilon^{\frac{7}{2}}\hbar^{-3}|\nu|$ which does not exceed $|\nu|=O(|Z-N|^{\frac{4}{3}})$. We leave easy details to the reader. □

Now we arrive to the lower estimate for E:

Corollary 25.4.3. *Let $N\asymp Z$. Then*

$$\mathsf{E}\ge \mathcal{E}^{\mathsf{TF}} + \mathsf{Scott} - CR \tag{25.4.14}$$

with R defined by (25.4.13).

Proof. We know from Subsection 25.2.1 that

$$\mathsf{E}\ge \mathsf{N}_1(H_W-\nu) + \nu N - \frac{1}{2}\mathsf{D}(\rho,\rho) - CZ^{\frac{5}{3}} \tag{25.4.15}$$

as W is given by (25.2.3). In virtue of Theorem 25.4.2

$$\mathsf{E}\ge \int \mathsf{Weyl}_1(x)\,dx + \nu\int \mathsf{Weyl}(x)\,dx - \frac{1}{2}\mathsf{D}(\rho,\rho) + \mathsf{Scott} - CR \tag{25.4.16}$$

[15)] From the point of view of generalization to the case when magnetic field is present and it is not too weak, so magnetic version of W^{TF} has multiple singularities.

where we also plugged instead of N as $N < Z$ (and $\nu < 0$)

$$N = \int \mathsf{Weyl}(x)\,dx \tag{25.4.17}$$

with

$$\mathsf{Weyl}(x) = \frac{q}{6\pi^2}\bigl(W(x)+\nu\bigr)_+^{\frac{3}{2}}. \tag{25.4.18}$$

One can check easily that three first terms in the right-hand expression of (25.4.18) constitute exactly $\Phi_*(W+\nu)$ coinciding with $\mathcal{E}^{\mathsf{TF}}$ as $W = W^{\mathsf{TF}}$.□

Remark 25.4.4. (i) As $a \le Z^{-\frac{1}{3}}$ using the same method one can prove a slightly better remainder estimate–with $Z^{\frac{3}{2}}a^{-\frac{1}{2}}$ replaced by

$$\sum_{1\le m<m'\le M} \min\Bigl((Z_m+Z_{m'})^{\frac{3}{2}}|\mathsf{x}_m-\mathsf{y}_{m'}|^{-\frac{1}{2}},\,(Z_m+Z_{m'})^2\Bigr) \tag{25.4.19}$$

allowing to lighter nuclei to be closer one to another.

(ii) To improve this estimate further, allowing lighter nuclei to be closer to heavier, ones one needs to improve Theorem 12.6.8 which seems to be too difficult task for a such little gain.

25.4.2 Upper Estimate for E

Recall that in virtue of Subsection 25.2.2

$$\mathsf{E} \le \mathsf{N}_1(H_W-\nu) + \nu N - \frac{1}{2}\mathsf{D}(\rho,\rho) + |\lambda_N-\nu|\cdot|\mathsf{N}(H_W-\nu)-N| + \frac{1}{2}\mathsf{D}(\operatorname{tr} e_N(x,x)-\rho,\operatorname{tr} e_N(x,x)-\rho) \tag{25.4.20}$$

and thus we need to estimate two last terms in the right-hand expression.

Estimating $|\lambda_N - \nu|$

First, we need to estimate $|\lambda_N-\nu|$. We will use the heuristic equality $\mathsf{N}(H_W-\lambda_N)\approx N$ or more precisely two inequalities

$$\mathsf{N}(H_W-\lambda_N-0) \le N \le \mathsf{N}(H_W-\lambda_N+0) \tag{25.4.21$_{1,2}$}$$

and equality

$$\int \mathsf{Weyl}(x)\,dx = \min(N,Z) \tag{25.4.22}$$

where the right inequality $(25.4.21)_2$ is valid only if $\lambda_N<0$ i.e. $\mathsf{N}(H_W)\ge N$.

Case $\lambda_N < \nu$. Then we will use $(25.4.21)_2$ and to calculate $\mathsf{N}(H_W - \lambda_N + 0)$ we will use semiclassical approximation:

$$\mathsf{N}(H_W - \lambda_N + 0) = \int \mathsf{Weyl}(x, \lambda_N)\, dx + O(R_0) \tag{25.4.23}$$

with the semiclassical error

$$R_0 = \int \zeta^2 \ell^{-1}\, dx \tag{25.4.24}$$

with the integral not exceeding

$$CZ \int_{\{|x|\le Z^{-\frac{1}{3}}\}} |x|^{-2}\, dx + C\int_{\{|x|\ge Z^{-\frac{1}{3}}\}} |x|^{-5}\, dx \asymp CZ^{\frac{2}{3}};$$

again we need to consider separately the case of $N \ge Z$ and $\nu = 0$, when integral (25.4.24) is taken over $\mathbb{R}^3$, and the case of $N < Z$ and $\nu < 0$, when this integral should be taken over $\{x\colon \ell(x) \le C(Z-N)^{-\frac{1}{3}}\}$; in the latter case to cover non-smoothness we consider an approximation (mollification) of W and an approximation error $\varepsilon^{\frac{7}{2}}\hbar^{-3} \ll 1$. Therefore

$$\int \mathsf{Weyl}(x, \lambda_N)\, dx \ge N - CZ^{\frac{2}{3}}. \tag{25.4.25}$$

Comparing with (25.4.22) we conclude that

$$\int \Bigl(\bigl(W(x)+\nu\bigr)_+^{\frac{3}{2}} - \bigl(W(x)+\lambda_N\bigr)_+^{\frac{3}{2}}\Bigr)\, dx \le CZ^{\frac{2}{3}}. \tag{25.4.26}$$

Here an integrand is non-negative (since $\lambda_N < \nu$). Further, one can see easily that the main contribution to this integral is delivered by the zone $\{x\colon \ell(x) \asymp |\lambda_N|^{-\frac{1}{4}}\}$ [16] and the whole integral is $\asymp |\lambda_N|^{-\frac{1}{4}}|\nu - \lambda_N|$. Therefore (25.4.26) yields that

$$|\lambda_N - \nu| \le C(|\nu| + |\lambda_N - \nu|)^{\frac{1}{4}} Z^{\frac{2}{3}},$$

which is equivalent to

$$|\lambda_N - \nu| \le CZ^{\frac{8}{9}} + C|\nu|^{\frac{1}{4}} Z^{\frac{2}{3}} \asymp CZ^{\frac{8}{9}} + C(Z-N)_+^{\frac{1}{3}} Z^{\frac{2}{3}} \le CZ. \tag{25.4.27}$$

In particular,

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[16] Provided $|\lambda_N| \le C_0 Z^{\frac{4}{3}}$. On the other hand, if $|\lambda_N| \ge C_0 Z^{\frac{4}{3}}$ one can see easily that (25.4.26) is $\asymp Z$ because $|\nu| \le c_0 Z^{\frac{4}{3}}$ due to $N \asymp Z$.

(25.4.28) If $|\nu|\le c_0Z^{\frac{8}{9}}$ (i.e. $(Z-N)_+\le c_1Z^{\frac{2}{3}}$), then $|\lambda_N|\le C_0Z^{\frac{8}{9}}$

and also

$$|\lambda_N-\nu|\cdot|\mathsf{N}(H_W-\nu)-N|\le CZ\cdot Z^{\frac{2}{3}}=CZ^{\frac{5}{3}}. \tag{25.4.29}$$

Case $\lambda_N\ge\nu$. Then we will use the left inequality $(25.4.21)_1$, but if $\mathsf{N}(H_W)<N$ then integral (25.4.24) is diverging.

To avoid all related difficulties we will consider first the case when we necessarily conclude that $|\lambda_N|\ge(1-\epsilon)|\nu|$. To do so observe that even if the main contribution to the integral (25.4.26)[17)] is delivered by the zone $\{x:\,\ell(x)\asymp(Z-N)|\lambda_N|^{-1}\asymp|\nu|^{\frac{3}{4}}|\lambda_N|^{-1}\}$, we will ignore this observation and consider a larger zone $\{x:\,\ell(x)\le C_0|\nu|^{-\frac{1}{4}}\}$ instead of $\{x:\,\ell(x)\le C_0|\nu|^{\frac{3}{4}}|\lambda_N|^{-1}\}$[18)].

One can prove easily that

(25.4.30) The contribution of the zone $\{x:\,\ell(x)\le C_0|\nu|^{-\frac{1}{4}}\}$ to the semiclassical remainder, when calculating $\mathsf{N}(H_W-\lambda_N)$, does not exceed $CZ^{\frac{2}{3}}$.

Therefore we arrive to the estimate

$$|\lambda_N-\nu|\le C|\nu|^{\frac{1}{4}}Z^{\frac{2}{3}}\asymp C(Z-N)_+^{\frac{1}{3}}Z^{\frac{2}{3}}\le CZ \tag{25.4.31}$$

(cf. (25.4.27)). In particular, we conclude that

(25.4.32) If $|\nu|\ge CZ^{\frac{8}{9}}$ (i.e. $(Z-N)\ge CZ^{\frac{2}{3}}$), then $|\lambda_N|\asymp|\nu|$

(cf. (25.4.28)). Then one can easily recover (25.4.27) completely. Since $|\mathsf{N}(H_W-\nu)-N|\le CZ^{\frac{2}{3}}$ we arrive to (25.4.29).

Case $|\nu|\le\eta=CZ^{\frac{8}{9}}$. This case (i.e. $(Z-N)\le\eta^{\frac{3}{4}}=CZ^{\frac{2}{3}}$) is the most important one. The easiest way to tackle it is to pick up ρ^{TF} and W^{TF} calculated as if $\nu=0$ i.e. $Z=N$; that means the change of the test function Ψ in the upper estimate.

We need to modify an upper estimate of $\sum_{1\le j\le N}\lambda_j$. To do this we note that

$$\lambda_N\ge-\eta \tag{25.4.33}$$

and

17) Now an integrand is non-positive.

18) Obviously these zones coincides as $|\nu|\asymp|\lambda_N|$.

(25.4.34) A number of eigenvalues between λ_N (if $\lambda_N < 0$) and 0 does not exceed $CZ^{\frac{2}{3}} + C\eta^{\frac{3}{4}}$,

which can be proven easily by our standard methods. Therefore

$$\sum_{1\le j\le N} \lambda_j \le \operatorname{Tr}(H_W^-) + C\eta\bigl(Z^{\frac{2}{3}} + \eta^{\frac{3}{4}}\bigr) \tag{25.4.35}$$

and the last term is less than $CZ^{\frac{5}{3}}$ as long as $\eta \le CZ^{\frac{20}{21}}$ which is fulfilled.

In this last case[19)] we arrive to an upper estimate with $\mathcal{E}^{\mathsf{TF}}$ calculated as if $\nu = 0$ i.e. $\mathcal{E}^{\mathsf{TF}}(\underline{Z};\underline{\mathsf{y}};Z)$ which is less than $\mathcal{E}^{\mathsf{TF}}(\underline{Z};\underline{\mathsf{y}};N)$. Actually the difference between these two is $\asymp |\nu|^{\frac{7}{4}} \le |\eta|^{\frac{7}{4}}$.

Estimating D-Term

We need to estimate the last term in the right-hand expression of (25.4.20); we estimate it by

$$\begin{aligned} &C_0\mathsf{D}\bigl(\operatorname{tr} e(x,x,\nu) - P'(W+\nu), \operatorname{tr} e(x,x,\nu) - P'(W+\nu)\bigr)\\ &\quad + C_0\mathsf{D}\bigl(\operatorname{tr} e(x,x,\nu) - \operatorname{tr} e_N(x,x), \operatorname{tr} e(x,x,\nu) - \operatorname{tr} e_N(x,x)\bigr)\\ &\qquad\qquad + C_0\mathsf{D}\bigl(\rho - P'(W+\nu), \rho - P'(W+\nu)\bigr), \end{aligned} \tag{25.4.36}$$

where the last term vanishes as $\rho = \rho^{\mathsf{TF}}$, $W = W^{\mathsf{TF}}$; however, for some technical reasons we want to avoid this assumption.

Estimating the First Term. To estimate the first term in (25.4.36) we apply the semiclassical asymptotics

$$\operatorname{tr} e(x,x,\nu) = \mathsf{Weyl}(x) + O(\zeta^2\ell^{-1}), \tag{25.4.37}$$

where $\mathsf{Weyl}(x) = P'(W(x)+\nu)$ and therefore this term does not exceed

$$\iint \zeta(x)^2\zeta(y)^2\ell(x)^{-1}\ell(y)^{-1}|x-y|^{-1}\,dxdy. \tag{25.4.38}$$

Estimating this integral by the double sum of the integrals over domains $\{(x,y)\colon \ell(x)\le Z^{-\frac{1}{3}}, \ell(y)\le Z^{-\frac{1}{3}}\}$ and $\{(x,y)\colon \ell(x)\ge Z^{-\frac{1}{3}}, \ell(y)\ge Z^{-\frac{1}{3}}\}$ we get

$$CZ^2\iint_{\{|x|\le Z^{-\frac{1}{3}},|y|\le Z^{-\frac{1}{3}}\}} |x|^{-2}|y|^{-2}|x-y|^{-1}\,dxdy \tag{25.4.39}$$

19) Pending an analysis of the next subsubsection.

and

$$C\iint_{\{|x|\ge Z^{-\frac{1}{3}},|y|\ge Z^{-\frac{1}{3}}\}} |x|^{-3}|y|^{-3}|x-y|^{-1}\,dxdy \tag{25.4.40}$$

respectively, and rescaling we get the same integrals but both with the "threshold" 1 rather than $Z^{-\frac{1}{3}}$ and both with factor $Z^{\frac{5}{3}}$ rather than Z^2 or 1 respectively; one can see easily that both obtained integrals (without factor $Z^{\frac{5}{3}}$) are $\asymp 1$. Therefore, expression (25.4.38) is $O(Z^{\frac{5}{3}})$.

Therefore we proved

Proposition 25.4.5. *As $W = W^{\mathsf{TF}}$ the first term in* (25.4.36) *does not exceed $CZ^{\frac{5}{3}}$.*

Remark 25.4.6. (i) For $N \ge Z$ and $\nu = 0$ we used that $\zeta \le C_1\ell^{-2}$ for $\ell \ge Z^{-\frac{1}{3}}$.

(ii) For $N < Z$ and $\nu < 0$ we used that zone $\{x\colon \ell \ge C(Z-N)^{-\frac{1}{3}}\}$ is classically forbidden ($W+\nu<0$ there) and therefore integral is taken over zone $\{x\colon \ell \le C(Z-N)^{-\frac{1}{3}}\}$ where $\zeta \le C_1\ell^{-2}$.

(iii) As $N < Z$ W^{TF} is not very smooth near $W+\nu=0$ but one can handle it by rescaling arguments.

(iv) Alternatively (preferably[15)]) one can replace W^{TF} by its mollification $W^{\mathsf{TF}}_{\varepsilon}$.

Remark 25.4.7. Estimating this term, and also the second D-term (in the next paragraph) we need to estimate the contribution of the singular zone $\{x\colon \ell(x) \le \bar{r} = Z^{-1}\}$ where effective semiclassical parameter is less than 1. We claim that there

$$e(x,x,\lambda) \le CZ^3 \qquad \text{for}\quad \lambda \le cZ^2. \tag{25.4.41}$$

Indeed, it is true if $\ell(x) \ge 1$. Also operator H is bounded from below by $-CZ^2$. And finally, in the ball of $B(\mathsf{y}_m, \epsilon Z^{-1})$ operator Δ is larger than $Z|x-\mathsf{y}_m|^{-1}$. We leave the easy details to the reader.

Therefore the contribution of this zone into N-term is $O(CZ^3\bar{r}^3) = O(1)$, into both D-terms is $O(Z^6\bar{r}^5) = O(Z)$, and into T-term is $O(Z^5\bar{r}^3) = O(Z^2)$.

Estimating the Second term. Consider now the second term in (25.4.36). Due to the arguments of the previous paragraph modulo $O(Z^{\frac{5}{3}})$ one can rewrite it as

$$C_1\mathsf{D}\bigl(P'(W+\lambda_N)-P'(W+\nu),\,P'(W+\lambda_N)-P'(W+\nu)\bigr). \tag{25.4.42}$$

Really, if we replace $\operatorname{tr} e(x,x,\nu)$ and $\operatorname{tr} e_N(x,x)$ by $\mathsf{Weyl}(x,\nu)$ and $\mathsf{Weyl}(x,\lambda_N)$ respectively we make a semiclassical errors estimated by $Z^{\frac{5}{3}}$ provided either $\lambda_N<\nu$ or $\lambda_N\asymp\nu$ which is always the case unless $|\nu|\le CZ^{\frac{8}{9}}$ but in this case we just "cheat" resetting everything to the case $\nu=0$.

Let us estimate (25.4.42). According to the previous Subsubsection 25.4.2.1 there are two cases:

(i) $N\ge Z-CZ^{\frac{2}{3}}$, in which case $|\nu|\le CZ^{\frac{8}{9}}$ and $|\lambda_N|\le CZ^{\frac{8}{9}}$, and (25.4.42) does not exceed

$$\begin{aligned}C|\nu-\lambda_N|^2\iint_{\{\ell(x)\le L,\ell(y)\le L\}}&|x-y|^{-1}\zeta(x)\zeta(y)\,dxdy\\ +C\iint_{\{\ell(x)\ge L,\ell(y)\ge L\}}&|x-y|^{-1}\zeta(x)^3\zeta(y)^3\,dxdy\end{aligned}$$

with $L=|\lambda_N-\nu|^{-\frac{1}{4}}$; one can calculate easily that both terms are of the magnitude $C|\lambda_N-\nu|^{\frac{7}{4}}\le CZ^{\frac{14}{9}}\ll Z^{\frac{5}{3}}$.

(ii) $N\le Z-CZ^{\frac{2}{3}}$, in which case (25.4.42) does not exceed

$$C|\nu-\lambda_N|^2\iint_{\{\ell(x)\le L,\ell(y)\le L\}}|x-y|^{-1}\zeta(x)\zeta(y)\,dxdy$$

with $L=|\nu|^{-\frac{1}{4}}$ and this integral does not exceed $|\lambda_N-\nu|^2|\nu|^{-\frac{1}{4}}$ which due to (25.4.27) does not exceed $C(Z-N)^{\frac{1}{3}}Z^{\frac{4}{3}}\le CZ^{\frac{5}{3}}$.

Estimating the Third term. The third term in (25.4.36) does not exceed

$$\begin{aligned}&C_1\mathsf{D}\bigl(\rho-\rho^{\mathsf{TF}},\rho-\rho^{\mathsf{TF}}\bigr)+\\ &\qquad C_1\mathsf{D}\bigl(P'(W+\nu)-P'(W^{\mathsf{TF}}+\nu),\,P'(W+\nu)-P'(W^{\mathsf{TF}}+\nu)\bigr)\end{aligned}$$

and we leave to the reader an easy proof that both terms here are $O(Z^{\frac{5}{3}-\delta})$ as W is a described mollification of W^{TF}.

Finally, a tTheorem

As we finished an upper estimate for E we arrive to the following main result:

Theorem 25.4.8. *Let $N\asymp Z$ and let Ψ be a ground state. Then*

$$|\mathsf{E}-\mathcal{E}^{\mathsf{TF}}-\mathsf{Scott}|\le C\begin{cases}Z^{\frac{5}{3}}+a^{-\frac{1}{2}}Z^{\frac{3}{2}} & \text{as}\quad a\ge Z^{-1},\\ Z^2 & \text{as}\quad a\le Z^{-1},\end{cases} \tag{25.4.43}$$

where a is the minimal distance between nuclei.

25.4.3 Improved Asymptotics

So far as $a \ge Z^{-\frac{1}{3}}$ we recovered only $O(Z^{\frac{5}{3}})$ for both error estimate in E and (as a coproduct, see Subsection 25.4.4) for $\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}}, \rho_\Psi - \rho^{\mathsf{TF}})$.

Our purpose is to improve them to $o(Z^{\frac{5}{3}})$ (or slightly better) as $a \gg Z^{-\frac{1}{3}}$ and recover the Schwinger and Dirac terms. To do so in the lower estimate for E one just need an improved electrostatic inequality (see Theorem 25.2.5) and also improved semiclassical estimates in $\operatorname{Tr}((H_W - \nu)^-)$ and $\mathsf{N}(H_W - \nu)$.

For the improved upper estimate we will need also to improve estimate $\frac{1}{2}\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}}, \mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}})$ for the test function Ψ and apply an estimate

$$|\frac{1}{2}\iint |x-y|^{-1} \operatorname{tr} e_N(x,y) e_N^\dagger(x,y)\, dxdy + \kappa_{\mathsf{Dirac}} \int \rho^{\mathsf{TF}\,\frac{4}{3}}(x)\, dx| \le Z^{\frac{5}{3}-\delta} \tag{25.4.44}$$

which is due to Theorem 6.4.17[20].

Remark 25.4.9. (i) Only contributions to the remainder of zones

$$\{x\colon Z^{-\frac{1}{3}-\delta_1} \le |x - \mathsf{y}_m| \le Z^{-\frac{1}{3}} b^{\delta_1}\} \tag{25.4.45}$$

with $b := \min(aZ^{\frac{1}{3}}, 1)$ (where now we assume that $b \ge 1$) should be considered because the contributions of both zones $\{x\colon \ell(x) \le Z^{-\frac{1}{3}} b^{-\delta_1}\}$ and $\{x\colon \ell(x) \le Z^{-\frac{1}{3}} b^{\delta_1}\}$ are $O(Z^{\frac{5}{3}} b^{-\delta})$.

(ii) Only m with $Z_m \ge Zb^{-\delta_2}$ should be considered because contributions of other m are are $O(Z^{\frac{5}{3}} b^{-\delta})$ as well.

Proposition 25.4.10. *Let ϑ be a (small) parameter such that $b^{-\delta_2} \le \vartheta \le 1$; consider m with $Z_m \ge Z\vartheta^{\delta_1}$. Let $\phi(x) = \psi(r^{-1}(x - \mathsf{y}_m))$ with $\psi \in \mathscr{C}_0^\infty(B(0,1))$ and r defined below.*

(i) Further, let $(Z-N)^{-\frac{1}{3}} \ge r = Z^{-\frac{1}{3}}\vartheta^{-1}$. Then inequalities

$$|\int \phi(x) \int_{-\infty}^{\lambda} \bigl(e(x,x,\lambda') - \mathsf{Weyl}(x,\lambda')\bigr)\, dx d\lambda' - \mathsf{Scott} - \mathsf{Schwinger}| \le CZ^{\frac{5}{3}}\vartheta^{\delta}, \tag{25.4.46}$$

[20] This theorem implies the above estimate with $\delta = 1$ which is definitely overkill for our purposes.

$$|\int \phi(x)\bigl(e(x,x,\lambda)-\mathsf{Weyl}(x,\lambda)\bigr)\,dx| \le CZ^{\frac{2}{3}}\vartheta^{\delta} \tag{25.4.47}$$

and

$$\mathsf{D}\Bigl(\phi\bigl(e(x,x,\lambda)-\mathsf{Weyl}(x,\lambda)\bigr),\phi\bigl(e(x,x,\lambda)-\mathsf{Weyl}(x,\lambda)\bigr)\Bigr)\le CZ^{\frac{5}{3}}\vartheta^{\delta} \tag{25.4.48}$$

hold with some exponent $\delta>0$ for all $\lambda\le 0$ and for ϕ which is r-admissible.

(ii) On the other hand, let $(Z-N)^{-\frac{1}{3}}\le r$. Let W be a constructed above mollification of W^{TF}. Then

(a) Estimates (25.4.46)–(25.4.48) *hold for all $\lambda\le\nu$.*

(b) Further, estimates (25.4.47), (25.4.48) *hold for $\lambda\in[\nu,0]$ such that $\mathsf{N}(H-\lambda)\le N$.*

(c) Furthermore, in this last case

$$|\lambda-\nu|\le CZ^{\frac{2}{3}}(Z-N)^{\frac{1}{3}}\vartheta^{\delta}. \tag{25.4.49}$$

To prove these statements we need to study behavior of the Hamiltonian trajectories. First we want to prove that in the indicated zone W^{TF} is a weak perturbation of W^{TF}_m which is a single atom Thomas-Fermi potential with Z_m and with $\nu_m=\nu$.

Proposition 25.4.11. *In the framework of Proposition 25.4.10 in $B(\mathsf{y}_m,r)$*

$$|D^{\alpha}(W^{\mathsf{TF}}-W^{\mathsf{TF}}_m)|\le c_{\alpha}W^{\mathsf{TF}}_m|x-\mathsf{y}_m|^{-|\alpha|}\vartheta^{\delta}. \tag{25.4.50}$$

This estimate holds for all α as $W^{\mathsf{TF}}/(-\nu)$ is disjoint from 1; otherwise it holds for $|\alpha|\le 3$ and

$$|D^{\alpha}(W^{\mathsf{TF}}-W^{\mathsf{TF}}_m)(x)-D^{\alpha}(W^{\mathsf{TF}}-W^{\mathsf{TF}}_m)(y)|\le cW^{\mathsf{TF}}_m|x-\mathsf{y}_m|^{-\frac{7}{2}}|x-y|^{\frac{1}{2}}\vartheta^{\delta} \tag{25.4.51}$$

for $|\alpha|=3$ and $|x-\mathsf{y}_m|\asymp|y-y_m|\asymp(Z-N)^{-\frac{1}{3}}$.

Proof. An easy proof based on the variational approach is left to the reader.□

Next, let us consider a manifold $\Sigma_\lambda = \{(x,\xi)\colon H(x,\xi)=\lambda\}$ with the classical Hamiltonian $H(x,\xi)=|\xi|^2-W(x)$, and let us introduce a measure $\upmu_\lambda$ with the density $dxd\xi : dH$ on Σ_λ; this measure is invariant with respect to the Hamiltonian flow with the Hamiltonian $H(x,\xi)$. Note that $\upmu_\lambda(\Sigma_\lambda)\asymp Z$.

Proposition 25.4.12. *In the framework of Proposition 25.4.10 there exists a set* $\Sigma'_{\lambda,\vartheta}\subset\Sigma_\lambda$ *such that*

$$\upmu_\lambda(\Sigma'_{\lambda,\vartheta})\le C\vartheta^\delta Z \tag{25.4.52}$$

and through each point (x,ξ) *belonging to* $\vartheta(Z^{-\frac{1}{3}},Z^{\frac{2}{3}})$*-vicinity of* $\Sigma_\lambda\setminus\Sigma'_{\lambda,\vartheta}$ *in* $T^*\mathbb{R}^3$ *there passes a Hamiltonian trajectory* $(x(t),\xi(t))$ *of* H *of the length* $T=Z^{-1}\vartheta^{-\delta}$ *along which*

$$\bigl|D^\alpha_{(xZ^{\frac{1}{3}},\xi Z^{-\frac{2}{3}})}\bigl(x(t)Z^{\frac{1}{3}},\xi(t)Z^{-\frac{2}{3}}\bigr)\bigr|\le C\vartheta^{-K}\qquad\forall\alpha:|\alpha|\le k \tag{25.4.53}$$

and

$$|x(t)-x(0)|Z^{\frac{1}{3}}+|\xi(t)-\xi(0)|Z^{-\frac{2}{3}}\ge\vartheta^K|t|Z, \tag{25.4.54}$$

where m *is arbitrary and* K,δ *depend on* k.

Proof. We will just sketch the proof.

(i) Consider first the case $M=1$. Then the the classical dynamical system is completely integrable since both the angular momentum and the energy are preserved.

First, let us include into $\Sigma'_{\lambda,\vartheta}$ all the points (x,ξ) with trajectories not residing over $\{\vartheta^{\delta'}Z^{-\frac{1}{3}}\le\ell(x)\le Z^{-\frac{1}{3}}\vartheta^{-\delta'}\}$ for all $t:|t|\le T$[21].

Further, if $(Z-N)_+\ge Z\vartheta^{\delta''}$ we also include into $\Sigma'_{\lambda,\vartheta}$ all the points (x,ξ) with the trajectories not residing over $B\bigl(\mathsf{y}_1,(1-\vartheta^{\delta'})\bar{r}\bigr)$; recall that for atoms $\bar{r}$ is an *exact* radius of $\operatorname{supp}(\rho^{\mathsf{TF}})$. Then (25.4.52)–(25.4.53) hold and we reduce δ,δ' if necessary.

It is known that not all the Hamiltonian trajectories are closed (see Appendix 25.A.2). Then one can prove easily that adding to $\Sigma'_{\lambda,\vartheta}$ the set satisfying (25.4.52) we can fulfill (25.4.52) and (25.4.54) as well[22]. One can find the similar arguments in the proof of Theorem 7.4.12.

[21] I.e. trajectories, leaving this "comfort zone" for some $t:|t|\le T$.

[22] It is important that in the classical dynamics is completely integrable.

(ii) The general case $M\geq 2$ is due of this particular one, Proposition 25.4.11 and trivial perturbation arguments. □

Proof of Proposition 25.4.10. Now estimates (25.4.46) and (25.4.47) follow from Propositions 25.4.11 and 25.4.12 and the standard arguments. Note that if $(Z-N)_+\geq Z\vartheta^{\delta''}$ we need to mollify W^{TF} in the standard way.

To prove estimate (25.4.48) we can use decomposition (16.4.1) and apply to the contribution of zone $\{(x,y)\colon |x-y|\geq Z^{-\frac{1}{2}}\vartheta^{\delta'}\}$ the same standard arguments. Meanwhile one can notice that the contribution of the zone $\{(x,y)\colon |x-y|\geq Z^{-\frac{1}{2}}\vartheta^{\delta'}\}$ is $O(Z^{\frac{5}{3}-\delta})$. □

Combining all these improvements we arrive to

Theorem 25.4.13. *Let $N\asymp Z$. Let $a\geq Z^{-\frac{1}{3}}$ and let Ψ be a ground state. Then*

$$|\mathsf{E}-\mathcal{E}^{\mathsf{TF}}-\mathsf{Scott}-\mathsf{Dirac}-\mathsf{Schwinger}|\leq CZ^{\frac{5}{3}}\bigl(Z^{-\delta}+(aZ^{\frac{1}{3}})^{-\delta}\bigr). \tag{25.4.55}$$

25.4.4 Corollaries and Discussion

Estimates for $\mathsf{D}(\rho_\Psi-\rho^{\mathsf{TF}},\rho_\Psi-\rho^{\mathsf{TF}})$

Recall that in the lower estimate there was in the left-hand expression a non-negative term $\frac{1}{2}\mathsf{D}(\rho_\Psi-\rho^{\mathsf{TF}},\rho_\Psi-\rho^{\mathsf{TF}})$ which we so far just dropped. Then in the frameworks of Theorems 25.4.8 and 25.4.13 we conclude that this term does not exceed the right-hand expressions of (25.4.43) and (25.4.55) respectively.

However, we can do better in the case $a\leq Z^{-\frac{1}{3}}$. Indeed, recall that the term $a^{-\frac{1}{2}}Z^{\frac{3}{2}}$ in the remainder estimate (25.4.43) appeared *only* because we replaced $\mathsf{Tr}((H_W-\nu)^-)$ by its Weyl approximation (with correction terms) which we by no means need for estimating this term since $\mathsf{Tr}((H_W-\nu)^-)$ was present in both lower and upper estimates. Then we arrive to the following

Theorem 25.4.14. *Let $N\asymp Z$ and let Ψ be a ground state. Then*

$$\mathsf{D}(\rho_\Psi-\rho^{\mathsf{TF}},\rho_\Psi-\rho^{\mathsf{TF}})\leq CQ:= C\left\{\begin{aligned} &Z^{\frac{5}{3}} && \textit{if}\quad a\leq Z^{-\frac{1}{3}},\\ &Z^{\frac{5}{3}}\bigl(Z^{-\delta}+(aZ^{\frac{1}{3}})^{-\delta}\bigr) && \textit{if}\quad a\geq Z^{-\frac{1}{3}}. \end{aligned}\right. \tag{25.4.56}$$

Estimates for Distance between Nuclei in the Free Nuclei Model

Let us estimate from below the distance between nuclei in the stable molecule in the free nuclei model (with the full energy optimized with respect to the position of the nuclei).

Theorem 25.4.15. *Let* $M \ge 2$ *and let condition* (25.3.33) *be fulfilled. Assume that*

$$\mathsf{E}(\underline{Z};\underline{\mathsf{y}};N) + \sum_{1\le m<m'\le M} Z_jZ_k|\mathsf{y}_m-\mathsf{y}_{m'}|^{-1} \le \min_{\substack{N_1,\dots,N_M:\\ N_1+\ldots+N_M=N}} \sum_{1\le m\le M} \mathsf{E}(Z_m;N_m) \tag{25.4.57}$$

Then

$$|\mathsf{y}_m-\mathsf{y}_{m'}| \ge Z^{-\frac{5}{21}+\delta_1} \qquad \forall m\ne m' \tag{25.4.58}$$

and

$$|\widehat{\mathsf{E}}^{\mathsf{TF}}(\underline{Z};N) - \widehat{\mathcal{E}}^{\mathsf{TF}}(\underline{Z};N) - \mathsf{Scott} - \mathsf{Dirac} - \mathsf{Schwinger}| \le CZ^{\frac{5}{3}-\delta}. \tag{25.4.59}$$

Proof. Note first that $|\mathsf{E}| \le CZ^{\frac{7}{3}}$ and in virtue of Theorem 25.4.8 we can replace E by $\mathcal{E}^{\mathsf{TF}}$ with $O(Z^2)$ error:

$$\mathcal{E}^{\mathsf{TF}}(\underline{Z};\underline{\mathsf{y}};N) + \sum_{1\le m<m'\le M} Z_jZ_k|\mathsf{y}_m-\mathsf{y}_{m'}|^{-1} \le \min_{\substack{N_1,\dots,N_M:\\ N_1+\ldots+N_M=N}} \sum_{1\le m\le M} \mathcal{E}^{\mathsf{TF}}(Z_m;N_m) - CZ^2; \tag{25.4.60}$$

which in virtue of Proposition 25.3.11 is impossible unless $a^{-7} \le CZ^2$ i.e. $a \ge \epsilon Z^{-\frac{2}{7}} \gg Z^{-\frac{1}{3}}$.

Then, again in virtue of Theorem 25.4.8 we can replace E by $\mathcal{E}^{\mathsf{TF}} + \mathsf{Scott}$ with $O(Z^{\frac{5}{3}})$ error. Let us take into account that for molecule Scott equals the sum of Scott_m. Therefore in (25.4.60) we can replace CZ^2 by $CZ^{\frac{5}{3}}$. Applying again Proposition 25.3.11 we conclude that $a \ge \epsilon Z^{-\frac{5}{21}}$.

Let us improve this estimate further. In virtue of Theorem 25.4.13 we can replace E by $\mathcal{E}^{\mathsf{TF}} + \mathsf{Scott} + \mathsf{Dirac} + \mathsf{Schwinger}$ with $O(Z^{\frac{5}{3}-\delta_2})$ error. However one needs to compare Dirac–Schwinger correction for the molecule with the sums of such corrections for separate atoms:

Proposition 25.4.16. *If* $a \ge Z^{-\frac{1}{3}+\delta_1}$ *and*

$$\mathcal{E}^{\mathsf{TF}}(\underline{Z};\underline{\mathsf{y}};N) = \sum_{1\le m\le M} \mathcal{E}^{\mathsf{TF}}(Z_m;N_m) + O(Z^{\frac{7}{3}-\delta_1}) \tag{25.4.61}$$

where $N = N_1 + ... + N_M$, *then*

$$\int (\rho^{\mathsf{TF}})^{\frac{4}{3}}\,dx = \sum_{1\le m\le M} \int (\rho^{\mathsf{TF}}_m)^{\frac{4}{3}}\,dx + O(Z^{\frac{5}{3}-\delta_2}), \tag{25.4.62}$$

where $\rho^{\mathsf{TF}}_m = \rho^{\mathsf{TF}}(x-\mathsf{y}_m;Z_m;N_m)$ *are atomic Thomas-Fermi densities.*

Proof of this Proposition 25.4.16 will be provided immediately. Therefore Dirac and $\mathsf{Schwinger}$ correction terms for a molecule are equal to the sums of Dirac_m and $\mathsf{Schwinger}_m$ correction terms respectively with $O(Z^{\frac{5}{3}-\delta_2})$ error and in (25.4.60) we can replace CZ^2 by $CZ^{\frac{5}{3}-\delta_2}$.

Applying Proposition 25.3.11 again we conclude that $a \ge Z^{\frac{5}{21}+\delta}$. □

Proof of Proposition 25.4.16. Note that the left-hand expression of (25.3.42) is equal to

$$\|\nabla\bigl(W^{\mathsf{TF}} - \bar{W}^{\mathsf{TF}}\bigr)\|^2 \qquad \text{with} \quad \bar{W}^{\mathsf{TF}} := \sum_{1\le m\le M} W^{\mathsf{TF}}_m \tag{25.4.63}$$

and therefore this expression is less than $CQ \le CZ^{\frac{7}{3}-\delta_1}$ as well. Then since $a \ge Z^{-\frac{1}{3}+\delta_1}$ we conclude that if we restrict the norm to the zone $\{x : |x-\mathsf{y}_m| \le Z^{-\frac{1}{3}+\delta}\}$, we can replace $\bar{\rho}^{\mathsf{TF}}$ and $\bar{W}^{\mathsf{TF}}$ by ρ^{TF}_m and W^{TF}_m respectively in (25.3.42), (25.4.63).

Using Thomas-Fermi equations we conclude that in this zone

$$|D^\alpha(W^{\mathsf{TF}} - W^{\mathsf{TF}}_m)| \le C_\alpha W^{\mathsf{TF}}_m \ell^{-|\alpha|} Z^{-\delta_2} \qquad \forall \alpha : |\alpha| \le 2 \tag{25.4.64}$$

and then $|(\rho^{\mathsf{TF}})^{\frac{4}{3}} - (\rho^{\mathsf{TF}}_m)^{\frac{4}{3}}| \le C(\rho^{\mathsf{TF}}_m)^{\frac{4}{3}} Z^{-\delta_2}$ which implies (25.4.62) because $\int (\rho^{\mathsf{TF}}_m)^{\frac{4}{3}}\,dx \asymp Z^{\frac{5}{3}}$ and contributions of zone $\{x : \ell(x) \ge Z^{-\frac{1}{3}+\delta}\}$ to each integral is $O(Z^{\frac{5}{3}-\delta})$. □

The following problem seems to be very challenging:

Problem 25.4.17. In the framework of the free nuclei model consider the case when assumption (25.3.33) is violated, i.e. when some nuclei are much lighter than the others. We do not need this assumption for

Theorems 25.4.8, 25.4.13 or 25.4.14 but we need to estimate from below the minimal distance between nuclei a.

We cannot do this without some generalization of Proposition 25.3.11, which we definitely do not expect to survive in its current form without assumption (25.3.33). It would be unrealistic to expect any estimate from below for $a_m := \min_{m'\neq m} |\mathsf{y}_m - \mathsf{y}_{m'}|$ without some estimate from below for Z_m.

The following problem seems to be reasonably challenging:

Problem 25.4.18. (i) Let us discuss the case $M = 2$ and $Z_2 \ll Z_1$, $a \le Z^{-\frac{1}{3}}$. Then there is an unpleasant remainder $O(a^{-\frac{1}{2}}Z^{\frac{3}{2}})$ in the trace asymptotics. Let us discuss how one can improve it.

Let us observe that in $\mathbb{R}^3 \setminus B(\mathsf{y}_1, Cb)$ we have $W_1^{\mathsf{TF}} \gg W_2^{\mathsf{TF}}$, where $b = \min(Z_2^{-\frac{1}{3}+\delta}, aZ_2Z^{-1})$. One can expect that we can modify W^{TF} in $B(\mathsf{y}_1, Cr_2)$ to W so that the dynamical systems corresponding to Hamiltonians H_W and H_{W_1} would be close; then for H_W we would be able to recover trace asymptotics with the remainder estimate $O(Z^{\frac{5}{3}-\delta})$.

Meanwhile, if $b \ge Z_2^{-1}$, i.e. $a \ge Z_2^{-2}Z$, the contribution of $B(\mathsf{y}_1, Cr_2)$ to the trace remainder would be $O(b^{-\frac{1}{2}}Z_2^{\frac{3}{2}}) = O(Z_2^{\frac{5}{3}-\delta}) + O(a^{-1/2}Z_2Z^{1/2})$ and we would improve $O(a^{-\frac{1}{2}}Z^{\frac{3}{2}})$ to $O(Z^{\frac{5}{3}-\delta} + a^{-\frac{1}{2}}Z_2Z^{\frac{1}{2}})$.

On the other hand, if $b \le Z_2^{-1}$, i.e. $a \le Z_2^{-2}Z$, the contribution of $B(\mathsf{y}_1, Cr_2)$ to the trace remainder would be $O(Z_2^2)$, so we would get the remainder $O(Z^{\frac{5}{3}-\delta} + Z_2^2)$.

In particular, we get $O(Z^{\frac{5}{3}-\delta})$ provided $Z_2 \le Z^{\frac{5}{6}-\delta}$.

(ii) Generalize for $M \ge 2$.

25.5 Negatively Charged sSystems

In this section we consider the case $N \ge Z$ and provide upper estimates for excessive negative charge $(N - Z)$ if $\mathsf{I}_N > 0$ and for ionization energy $\mathsf{I}_N := \mathsf{E}_{N-1} - \mathsf{I}_N$.

25.5.1 Estimates of the Correlation Function

First of all, we provide some estimates which will be used for both negatively and positively charged systems. Let us consider the ground-state function $\Psi(x_1, \varsigma_1; \dots ; x_N, \varsigma_N)$ and the corresponding density $\rho_\Psi(x)$.

The crucial role plays estimate (25.4.56) $\mathsf{D}\bigl(\rho_\psi-\rho^{\mathsf{TF}},\rho_\psi-\rho^{\mathsf{TF}}\bigr)\le CQ$ of Theorem 25.4.14 and the difference between upper and lower bounds for E_N (with $\mathsf{N}_1(H_W-\nu)+\nu N$ not replaced by its semiclassical approximation).

Let us consider the *classical density* of the electron system

$$\varrho_{\underline{x}}(x)=\sum_{1\le j\le N}\delta(x-x_j) \tag{25.5.1}$$

and the *smeared classical density*

$$\varrho_{\underline{x},\varepsilon}(x)=\varrho_{\underline{x}}*\phi_\varepsilon=\sum_{1\le j\le N}\phi_\varepsilon(x-x_j) \tag{25.5.2}$$

where ε will be chosen later; here $(\underline{x},\underline{\varsigma})=(x_1,\varsigma_1;\ldots,x_N,\varsigma_N)\in(\mathbb{R}^3\times\mathbb{C}^q)^N$,

(25.5.3) $\phi_\varepsilon(z)=\varepsilon^{-3}\phi(z\varepsilon^{-1})$, $\phi\in\mathscr{C}_0^\infty\bigl(B(0,\frac{1}{2})\bigr)$ is a spherically symmetric, non-negative function such that $\int\phi(x)\,dx=1$.

Then $\int\phi_\varepsilon(x)f(x)\,dx=f(0)+O(\varepsilon^2)$ for any $f\in\mathscr{C}^2$. Let us consider

$$K_N(\underline{x})\coloneqq\frac{1}{2}\mathsf{D}\bigl(\varrho_{\underline{x}}(\cdot)-\rho(\cdot),\varrho_{\underline{x}}(\cdot)-\rho(\cdot)\bigr) \tag{25.5.4}$$

where $\rho=\frac{1}{4\pi}\Delta(W-V)$, W is either W^{TF} if $\nu=0$ or a "good" approximation for it, constructed in the previous section.

Using Newton's screening theorem[23)] we conclude that

$$\sum_{1\le j<k\le N}|x_j-x_k|^{-1}\ge\frac{1}{2}\mathsf{D}\bigl(\varrho_{\underline{x}}(\cdot),\varrho_{\underline{x}}(\cdot)\bigr)-C\varepsilon^{-1}N \tag{25.5.5}$$

where the last term estimates

$$\sum_{1\le j\le N}\mathsf{D}\bigl(\phi_\varepsilon(x-x_j),\phi_\varepsilon(x-x_j)\bigr).$$

On the other hand,

$$\frac{1}{2}\mathsf{D}\bigl(\varrho_{\underline{x}}(\cdot),\varrho_{\underline{x}}(\cdot)\bigr)=\int\varrho_{\underline{x}}(|x|^{-1}*\rho)\,dx+K_N(\underline{x})-\frac{1}{2}\mathsf{D}(\rho,\rho) \tag{25.5.6}$$

23) That uniformly charged sphere $S(0,r)$ creates potential $v(x)=-q\min(|x|^{-1},r^{-1})$ where q is the total charge of the sphere.

and therefore

$$\mathsf{H}_N \ge \sum_{1\le j\le N} H_{W_\varepsilon}(x_j) + K_N(\underline{x}) - \frac{1}{2}\mathsf{D}(\rho,\rho) - C\varepsilon^{-1}N \tag{25.5.7}$$

on $(\mathscr{L}^2(\mathbb{R}^3,\mathbb{C}^q))^N$ where W_ε is the *smeared potential*:

$$W_\varepsilon(x) = V(x) - \phi_\varepsilon * |x|^{-1} * \rho. \tag{25.5.8}$$

Observe that the smeared potential does not depend on $\underline{x}$ and is defined via ρ rather than ρ_Ψ.

Also let us define

$$N_x(x_2,\ldots,x_N) := \sum_{2\le j\le N} (\chi_x * \phi_\varepsilon)(x_j) \tag{25.5.9}$$

and

$$\bar{N}_x := \int \rho(y)\chi_x(y)\,dy \tag{25.5.10}$$

with $\chi_x(y) := \chi(x,y)$, $\chi\in\mathscr{C}^\infty(\mathbb{R}^6)$.

Furthermore, let us consider function $\theta\in\mathscr{C}^\infty(\mathbb{R}^3)$ such that

$$0\le\theta\le 1. \tag{25.5.11}$$

Finally, consider

$$\mathcal{J} := \Bigl|\int \Bigl(\rho^{(2)}_\Psi(x,y) - \rho(y)\rho_\Psi(x)\Bigr)\theta(x)\chi(x,y)\,dxdy\Bigr|. \tag{25.5.12}$$

Obviously

$$\begin{aligned}
\mathcal{J} \le \int \rho^{(2)}_\Psi(x,y)\bigl|\chi_x*\phi_\varepsilon - \chi_x(y)\bigr|\theta(x)\,dxdy\\
+ N\int |\Psi(x,x_2,\ldots,x_N)|^2\bigl|N_x(x_2,\ldots,x_N) - \bar{N}_x\bigr|\theta(x)\,dxdx_2\cdots dx_N\\
\le CN\varepsilon^s\|\nabla_y^{s+1}\chi\|_{\mathscr{L}^\infty}\Theta\\
+\Bigl(N\int |\Psi(x,x_2,\ldots,x_N)|^2|N_x-\bar{N}_x|^2\theta(x)\,dxdx_2\cdots dx_N\Bigr)^{\frac{1}{2}}\Theta^{\frac{1}{2}}
\end{aligned}$$

where $\rho^{(2)}_\Psi(\cdot,\cdot)$ is the *quantum correlation function,*

$$\rho^{(2)}_\Psi(x,y) := N(N-1)\int |\Psi(x,y,x_3,\dots,x_N)|^2\,dx_3\cdots dx_N, \tag{25.5.13}$$

$$\int \rho^{(2)}_\Psi(x,y)dy = (N-1)\rho_\Psi(x), \tag{25.5.14}$$

$$\Theta=\Theta_\Psi := \int \theta(x)\rho_\Psi(x)dx \tag{25.5.15}$$

and we used Cauchy-Schwartz inequality.

Since

$$N_x(x_2,\dots,x_N)-\bar{N}_x = \int \bigl(\sum_{2\le j\le N}\phi_\varepsilon(y-x_j)-\rho(y)\bigr)\chi(x,y)\,dxdy, \tag{25.5.16}$$

we again from Cauchy-Schwartz inequality conclude that

$$\bigl|N_x-\bar{N}_x|^2 \le C\|\nabla_y\chi\|^2_{\mathscr{L}^2}\cdot K_{N-1}(x_2,\dots,x_N). \tag{25.5.17}$$

Note that

$$\sum_{1\le j\le N}\langle \mathsf{H}_N\theta^{\frac12}(x_j)\Psi,\theta^{\frac12}(x_j)\Psi\rangle = \\ \mathsf{E}_N\int\int \theta(x)\rho_\Psi(x)\,dx + \int |\nabla\theta^{\frac12}|^2(x)\rho_\Psi(x)\,dx \tag{25.5.18}$$

and then (25.5.7) yields that

$$\mathsf{E}_N\int\theta(x)\rho_\Psi(x)\,dx \ge -\int |\nabla\theta^{\frac12}|^2(x)\rho_\Psi(x)\,dx \\ + \sum_{1\le j,k\le N}\langle H_{W_\varepsilon}(x_k)\theta^{\frac12}(x_j)\Psi,\theta(x_j)\Psi\rangle \\ +\int K_N(\underline{x})\theta(x_1)|\Psi(x_1,\dots,x_N)|^2\,dx_1\dots dx_N - \frac12\mathsf{D}(\rho,\rho)\Theta - C\varepsilon^{-1}N\Theta. \tag{25.5.19}$$

Also note that

(25.5.20) The sum of $(N-1)$ lowest eigenvalues of H_{W_ε} on $\mathcal{H}$ is greater than $\bigl(\nu N + \mathsf{N}_1(H_{W_\varepsilon}-\nu)\bigr)$.

Then the second term in the right-hand expression of (25.5.19) is bounded from below by $\bigl(\nu N+\mathsf{N}_1(H_{W_\varepsilon}-\nu)\bigr)\Theta$, while the left-hand expression is $\mathsf{E}_N\Theta$. Therefore assembling terms proportional to Θ we conclude that

$$S\Theta + \int |\nabla \theta^{\frac{1}{2}}|^2 \rho_\Psi\, dx \ge \sum_j \langle H_{W_\varepsilon, x_j} \theta^{\frac{1}{2}}(x_j)\Psi, \theta^{\frac{1}{2}}(x_j)\Psi\rangle \\ + N\int K_N(x_1,\dots,x_N)\theta(x_1)|\Psi(x_1,\dots,x_N)|^2\, dx_1\cdots dx_N \tag{25.5.21}$$

with

$$S := \mathsf{E}_N - \nu N - \mathsf{N}_1(H_{W_\varepsilon} - \nu) + \frac{1}{2}\mathsf{D}(\rho,\rho). \tag{25.5.22}$$

Due to the non-negativity of operator D_x^2, the last term in (25.5.21) is greater than $-CT\Theta$ with

$$T = \sup_{\operatorname{supp}(\theta)} W; \tag{25.5.23}$$

so we arrive to

$$N\int K_N(x_1,\dots,x_N)\theta(x_1)|\Psi(x_1,\dots,x_N)|^2\, dx_1\cdots dx_N \le \\ C\bigl(S + T + \varepsilon^{-1}N\bigr)\Theta + P \tag{25.5.24}$$

with

$$P = \int |\nabla\theta^{\frac{1}{2}}|^2\rho_\Psi\, dx. \tag{25.5.25}$$

Combining this inequality with (25.5.13), (25.5.17) we conclude that

$$\mathcal{J} \le C\sup_x \|\nabla_y \chi_x\|_{\mathscr{L}^2(\mathbb{R}^3)} \Bigl(\bigl(S + \varepsilon^{-1}N + T\bigr)\Theta + P\Bigr)^{\frac{1}{2}}\Theta^{\frac{1}{2}} \\ + C\varepsilon N\|\nabla_y\chi\|_{\mathscr{L}^\infty}\Theta \tag{25.5.26}$$

due to obvious estimate

$$K_{N-1}(x_2,\dots,x_N) \le 2K_N(x_1,\dots,x_N) + \varepsilon^{-1}N. \tag{25.5.27}$$

Now we want to estimate S from above and for this we need an upper estimate for E_N. Recall that due to the arguments of Subsection 25.2.2 $S \le CQ$ provided we manage to prove that

(25.5.28) Expressions (25.2.23)–(25.2.26) satisfy the same estimates as before if we plug W_ε instead of W.

So, we need to calculate both semiclassical errors (which are calculated exactly as for $W = W^{\mathsf{TF}}$) and the principal parts, and in calculations of

$$\mathsf{D}\bigl(P'(W_\varepsilon+\nu)-\rho^{\mathsf{TF}}, P'(W_\varepsilon+\nu)-\rho^{\mathsf{TF}}\bigr) \tag{25.5.29}$$

and

$$\mathsf{D}(\rho_\varepsilon-\rho^{\mathsf{TF}}, \rho_\varepsilon-\rho^{\mathsf{TF}}) \tag{25.5.30}$$

an error is $O(\varepsilon^2 Z^3)$ due to estimates

$$|D^\alpha (W-W_\varepsilon)| \le \\ C\begin{cases} Z\ell^{-1-|\alpha|}(1+\ell\varepsilon^{-1})^{-2} & \forall\alpha & \text{if } \ \ell\le \epsilon Z^{-\frac{1}{3}}\\ \varepsilon^2\ell^{-6-|\alpha|} & \forall\alpha & \text{if } \ \ell\ge \epsilon Z^{-\frac{1}{3}}, \ell\not\asymp \bar{r},\\ \varepsilon^2\ell^{-6-|\alpha|} & \forall\alpha: |\alpha|\le \dfrac{3}{2} & \text{if } \ \ell\asymp \bar{r}. \end{cases} \tag{25.5.31}$$

Then one can prove easily that the sum of these two expressions (25.5.29) and (25.5.30) does not exceed $CQ+CZ^3\varepsilon^2+CZ^2\varepsilon$, and this estimate cannot be improved. Choosing $\varepsilon\le Z^{-\frac{2}{3}}$ we estimate these two terms by $CZ^{\frac{5}{3}}$.

Under this restriction a smearing error in the principal part of the asymptotics of $\int e(x,x,\lambda)\,dx$, namely

$$|\int \bigl(P'(W_\varepsilon+\nu)-P'(W+\nu)\bigr)\,dx|, \tag{25.5.32}$$

does not exceed $CZ^{\frac{3}{2}}\varepsilon^{\frac{3}{2}}=O(Z^{\frac{1}{2}})$ which is less than the semiclassical error. Then $S\le CQ$.

So, the following proposition is proven:

Proposition 25.5.1. *If θ,χ are as above then*

$$\mathcal{J}=|\int \Bigl(\rho^{(2)}_\Psi(x,y)-\rho(y)\rho_\Psi(x)\Bigr)\theta(x)\chi(x,y)\,dxdy|\le \\ C\sup_x \|\nabla_y\chi_x\|_{\mathscr{L}^2(\mathbb{R}^3)}\Bigl((Q+\varepsilon^{-1}N+T)^{\frac{1}{2}}\Theta + P^{\frac{1}{2}}\Theta^{\frac{1}{2}}\Bigr)+C\varepsilon N\|\nabla_y\chi\|_{\mathscr{L}^\infty}\Theta \tag{25.5.33}$$

with $\Theta=\Theta_\Psi$ defined by (25.5.15) *and T,P defined by* (25.5.23), (25.5.25) *respectively and arbitrary $\varepsilon\le Z^{-\frac{2}{3}}$.*

25.5.2 Excessive Negative Charge

Let us select $\theta=\theta_b$

$$\operatorname{supp}(\theta)\subset\{x:\ \ell(x)\ge b\}. \tag{25.5.34}$$

Observe that $\mathsf{H}_N\Psi=\mathsf{E}_N\Psi$ yields

$$\mathsf{E}_N\int \rho_\Psi(x)\ell(x)\theta(x)\,dx=\sum_j \langle \Psi,\ell(x_j)\theta(x_j)\mathsf{H}_N\Psi\rangle = \\ \sum_j \langle \ell(x_j)^{\frac{1}{2}}\theta^{\frac{1}{2}}(x_j)\Psi, \ell(x_j)^{\frac{1}{2}}\theta^{\frac{1}{2}}(x_j)\mathsf{H}_N\Psi\rangle - \sum_j \|\nabla\bigl(\theta^{\frac{1}{2}}(x_j)\ell(x_j)^{\frac{1}{2}}\bigr)\Psi\|^2 \tag{25.5.35}$$

and isolating the contribution of j-th electron in j-th term we get

$$\mathsf{E}_N\int \rho_\Psi(x)\ell(x)\theta\,dx \ge \mathsf{E}_{N-1}\int \rho_\Psi(x)\ell(x)\theta(x)\,dx + \\ \sum_j \langle \Psi,\ell(x_j)\theta(x_j)\Bigl(-V(x_j)+\sum_{k:k\ne j}|x_j-x_k|^{-1}\Bigr)\Psi\rangle - \sum_j \|\nabla\bigl(\theta^{\frac{1}{2}}(x_j)\ell(x_j)^{\frac{1}{2}}\bigr)\Psi\|^2 \tag{25.5.36}$$

due to non-negativity of operator D_x^2.

Now let us select b to be able to calculate the magnitude of Θ. Observe that

$$|\int \theta(x)\bigl(\rho_\Psi(x)-\rho(x)\bigr)\,dx| \le C\mathsf{D}(\rho_\Psi-\rho,\rho_\Psi-\rho)^{\frac{1}{2}}\|\nabla\theta^{\frac{1}{2}}\| \asymp \\ C\mathsf{D}(\rho_\Psi-\rho,\rho_\Psi-\rho)^{\frac{1}{2}}b^{\frac{1}{2}} \le CQ^{\frac{1}{2}}b^{\frac{1}{2}} \tag{25.5.37}$$

and

$$\int \theta(x)\rho(x)\,dx \asymp b^{-3} \tag{25.5.38}$$

as long as

$$Z^{-\frac{1}{3}} \le b \le \epsilon(Z-N)_+^{-\frac{1}{3}} \tag{25.5.39}$$

because $\rho\asymp |x|^{-6}$ as $Z^{-\frac{1}{3}}\le |x|\le c_0(Z-N)_+^{-\frac{1}{3}}$. Note that the right-hand expression of (25.5.38) is larger than the right-hand expression of (25.5.37) as $b\ge C_0Q^{-\frac{1}{7}}$. Therefore let us pick up

$$b:=\epsilon_0 Q^{-\frac{1}{7}}; \tag{25.5.40}$$

it does not conflict with (25.5.39) provided

$$N\ge Z-C_0Q^{\frac{3}{7}} \tag{25.5.41}$$

and then

$$\Theta \asymp Q^{\frac{3}{7}}. \tag{25.5.42}$$

Then the same arguments imply that the last term in the right-hand expression of (25.5.36) does not exceed $Cb^{-1}\Theta$; using inequality

$$\int \rho_\Psi(x)\ell(x)\theta(x)dx \ge b\Theta \tag{25.5.43}$$

we conclude that

$$\begin{aligned} b\mathsf{I}_N\Theta_b \le \int \theta(x)V(x)\ell(x)\rho_\Psi(x)\,dx \\ - \int \rho^{(2)}_\Psi(x,y)\ell(x)|x-y|^{-1}\theta(x)\,dxdy + Cb^{-1}\Theta = \\ = \int \theta(x)V(x)\ell(x)\rho_\Psi(x)\,dx \\ - \int \rho^{(2)}_\Psi(x,y)\ell(x)|x-y|^{-1}\bigl(1-\theta(y)\bigr)\theta(x)\,dxdy \\ - \int \rho^{(2)}_\Psi(x,y)\ell(x)|x-y|^{-1}\theta(y)\theta(x)\,dxdy + Cb^{-1}\Theta. \end{aligned} \tag{25.5.44}$$

Denote by $\mathcal{I}_1$, $\mathcal{I}_2$, and $\mathcal{I}_3$ the first, second and third terms in the right-hand expression of (25.5.44) respectively. Symmetrizing $\mathcal{I}_3$ in the right-hand expression of (25.5.44) with respect to x and y we see that

$$\mathcal{I}_3 = -\frac{1}{2}\int \rho^{(2)}_\Psi(x,y)\bigl(\ell(x)+\ell(y)\bigr)|x-y|^{-1}\theta(y)\theta(x)\,dxdy$$

and using inequality $\ell(x)+\ell(y)\ge \min_j(|x-\mathsf{y}_j|+|y-\mathsf{y}_j|)\ge |x-y|$ we conclude that this term is less than

$$\begin{aligned} -\frac{1}{2}\int \rho^{(2)}_\Psi(x,y)\theta(y)\theta(x)\,dxdy = \\ -\frac{1}{2}(N-1)\int \rho_\Psi(x)\theta(x)\,dx + \frac{1}{2}\int \rho^{(2)}_\Psi(x,y)\bigl(1-\theta(y)\bigr)\theta(x)\,dxdy. \end{aligned} \tag{25.5.45}$$

Here the first term is exactly $-\frac{1}{2}(N-1)\Theta$; replacing $\rho^{(2)}_\Psi(x,y)$ by $\rho(y)\rho_\Psi(x)$ we get

$$\frac{1}{2}\int \bigl(1-\theta(y)\bigr)\rho(y)\,dy \times \Theta \tag{25.5.46}$$

with an error

$$\frac{1}{2}\int \bigl(\rho^{(2)}_\Psi (x,y)-\rho(y)\rho_\Psi(x)\bigr)\bigl(1-\theta(y)\bigr)\theta(x)\,dxdy \tag{25.5.47}$$

which we estimate using Proposition 25.5.1 with $\chi(x,y)=1-\theta(y)$. Then $\|\nabla_y\chi_x\|_{\mathscr{L}^2}\asymp b^{\frac{1}{2}}$, $\|\nabla_y\chi\|_{\mathscr{L}^\infty}\asymp b^{-1}$, $T\asymp b^{-4}$, $P\asymp b^{-1}\Theta$ and picking up $\varepsilon=Z^{-\frac{2}{3}}$ we conclude that an error (25.5.47) is less than $Cb^{\frac{1}{2}}Q^{\frac{1}{2}}\Theta\asymp CQ^{\frac{3}{7}}\Theta$ and then we conclude that

$$\mathcal{I}_3\le -\frac{1}{2}(N-Z)_+\Theta + CQ^{\frac{3}{7}}\Theta \tag{25.5.48}$$

because $\int\rho\theta\,dy\asymp Q^{\frac{3}{7}}$ and $\int\rho(y)\,dy=\min(Z,N)$.

On the other hand,

$$\mathcal{I}_2\le -\int \rho^{(2)}_\Psi (x,y)\ell(x)|x-y|^{-1}\bigl(1-\bar\theta(y)\bigr)\theta(x)\,dxdy \tag{25.5.49}$$

with $\bar\theta=\theta_{b(1-\epsilon)}$ and replacing $\rho^{(2)}_\Psi(x,y)$ by $\rho(y)\rho_\Psi(x)$ we get

$$-\int \rho_\Psi(x)\rho(y)\ell(x)|x-y|^{-1}\bigl(1-\bar\theta(y)\bigr)\theta(x)\,dxdy \tag{25.5.50}$$

and we estimate an error in the same way by $CQ^{\frac{3}{7}}\Theta$.

Therefore

$$\begin{aligned}\mathcal{I}_1+\mathcal{I}_2 \le \int \theta(x)V(x)\ell(x)\rho_\Psi(x)\,dx - {}\\ \int \rho_\Psi(x)\ell(x)\rho(y)|x-y|^{-1}\bigl(1-\bar\theta(y)\bigr)\theta(x)\,dxdy + CQ^{\frac{3}{7}}\Theta = {}\\ \int \theta(x)W(x)\ell(x)\rho_\Psi(x)\,dx\\ +\int \rho(y)\rho_\Psi(x)\ell(x)|x-y|^{-1}\bar\theta(y)\theta(x)\,dxdy + CQ^{\frac{3}{7}}\Theta\end{aligned} \tag{25.5.51}$$

due to $V-W=|x|^{-1}*\rho$. Since $W\ell\le Cb^{-3}$ we can skip the first term in the right-hand expression. Furthermore, as

$$\int \rho(y)|x-y|^{-1}\bar\theta(y)\,dy\asymp\Theta\asymp Q^{\frac{3}{7}} \tag{25.5.52}$$

we can skip the second term as well.

Adding $\mathcal{I}_3$ to and multiplying by Θ^{-1} we arrive to

$$b\mathsf{I}_N \le -\frac{1}{2}(N-Z)_+ + CQ^{\frac{3}{7}} \tag{25.5.53}$$

which implies immediately

Theorem 25.5.2. *Let condition* (25.3.33) *be fulfilled.*

(i) In the fixed nuclei model let $\mathsf{I}_N > 0$. *Then*

$$(N-Z)_+ \le CQ^{\frac{3}{7}} = CZ^{\frac{5}{7}} \begin{cases} 1 & \textit{if}\ \ a\le Z^{-\frac{1}{3}},\\ Z^{-\delta}+(aZ^{\frac{1}{3}})^{-\delta} & \textit{if}\ \ a\ge Z^{-\frac{1}{3}}. \end{cases} \tag{25.5.54}$$

(ii) In particular, for a single atom and for molecule with $a\ge Z^{-\frac{1}{3}+\delta}$

$$(N-Z)_+ \le Z^{\frac{5}{7}-\delta'}. \tag{25.5.55}$$

(iii) In the free nuclei model let $\widehat{\mathsf{I}}_N > 0$. *Then estimate* (25.5.55) *holds.*

25.5.3 Estimate for Ionization Energy

Recall that as $N<Z$ we assumed that $N\ge Z-CQ^{\frac{3}{7}}$ (see (25.5.41)) and $b=Q^{-\frac{1}{7}}$. Then (25.5.53) also implies $\mathsf{I}_N\le CQ^{\frac{4}{7}}$ and we arrive to

Theorem 25.5.3. *Let condition* (25.3.33) *be fulfilled and let* $N\ge Z-C_0Z^{\frac{5}{7}}$. *Then*

(i) In the framework of fixed nuclei model

$$\mathsf{I}_N \le CZ^{\frac{20}{21}}. \tag{25.5.56}$$

(ii) In the framework of free nuclei model with $N\ge Z-C_0Z^{\frac{5}{7}-\delta}$

$$\widehat{\mathsf{I}}_N \le Z^{\frac{20}{21}-\delta'}. \tag{25.5.57}$$

Remark 25.5.4. (i) Classical theorem of G. Zhislin [1] implies that the system can bind at least Z electrons; the proof is based on the demonstration that the energy of the system with $N<Z$ electrons plus one electron on the distance r is increasing as $r\to+\infty$ because potential created by the system with $N<Z$ electrons behaves as $(Z-N)|x|^{-1}$ as $|x|\to\infty$;

(ii) In the proof of Theorem 25.5.2(iii) and 25.5.3(ii) we note that tearing of one electron in free nuclei model is easier than in the fixed nuclei model.

The following problem does not look extremely challenging:

Problem 25.5.5. In Theorems 25.5.2(i),(ii) and 25.5.3(i) get rid of condition (25.3.33).

25.6 Positively Charged sSystems

In this section we consider the case of positively charged system with $Z - N \ge C_0 Q^{\frac{3}{7}}$ with sufficiently large C_0.

First let us find asymptotics of the ionization energy; the principal term will be $-\nu$ but we need to estimate a remainder.

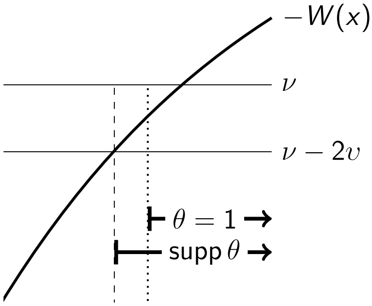
25.6.1 Estimate from above for Ionization Energy

As $M = 1$ construction is well-known: let us pick up function θ such that $\theta = 1$ as $|x - y_m| \ge \bar{r} - \beta$ and $\theta = 0$ as $|x - y_m| \le \bar{r} - 2\beta$ where $\bar{r}$ is an exact radius of support ρ^{TF}. Here $\beta \ll \bar{r}$. As $M \ge 1$ let us pick instead

$$\theta(x) = f^2\bigl(\upsilon^{-1}[W(x) + \nu]\bigr) \tag{25.6.1}$$

where $f \in \mathscr{C}^\infty(\mathbb{R})$, supported in $(-\infty, 2)$ and equal 1 in $(-\infty, 1)$, $\upsilon \le \nu$.

We will assume that



$$a \ge \bar{r} = C_1 (Z - N)^{-\frac{1}{3}} \tag{25.6.2}$$

with sufficiently large C_1; we will discuss dropping this assumption later. Then as we know that ρ^{TF} is supported in $c\bar{r}$-vicinity of nuclei, we conclude that "atoms" are rather disjoint.

One can see easily that then as $W + \nu \approx 0$,

$$|\nabla W| \asymp \bar{r}^{-5}; \tag{25.6.3}$$

then the width of the zone $\{x \colon 0 \le W(x) + \nu \le 2\upsilon\}$ is $\asymp \upsilon |\nabla W|^{-1} \asymp \beta = \upsilon \bar{r}^5$ and

$$\Theta^{\mathsf{TF}} := \int \theta(x)\rho^{\mathsf{TF}}\,dx \asymp \upsilon^{\frac{3}{2}} \times \beta\bar{r}^2 = \upsilon^{\frac{5}{2}}\bar{r}^7 \tag{25.6.4}$$

while $\|\nabla\theta\| \asymp \beta^{-\frac{1}{2}}\bar{r} = \upsilon^{-\frac{1}{2}}\bar{r}^{-\frac{3}{2}}$ and therefore to ensure that Θ has the same magnitude (25.6.4) we pick up the smallest υ such that $\upsilon^{\frac{5}{2}}\bar{r}^7 \ge C\upsilon^{-\frac{1}{2}}\bar{r}^{-\frac{3}{2}}Q^{\frac{1}{2}}$ i.e.

$$\upsilon := C_2\bar{r}^{-\frac{17}{6}}Q^{\frac{1}{6}} \qquad (\iff \beta = C_2\bar{r}^{\frac{13}{6}}Q^{\frac{1}{6}}); \tag{25.6.5}$$

then

$$\Theta \asymp \bar{r}^{-\frac{1}{12}}Q^{\frac{5}{12}} \tag{25.6.6}$$

Then (25.5.15) is fulfilled. Note that $\upsilon \le \nu = \bar{r}^{-4}$ iff $(Z-N) \ge Q^{\frac{3}{7}}$ exactly as we assumed.

Then (25.5.44) is replaced by

$$\begin{aligned}\mathsf{I}_N \int \ell(x)\rho_\Psi(x)\theta(x)\,dx \le \int \theta(x)V(x)\ell(x)\rho_\Psi(x)\,dx\\ - \int \rho^{(2)}_\Psi(x,y)\ell(x)|x-y|^{-1}\theta(x)\,dxdy + C\beta^{-2}\bar{r}\Theta\end{aligned} \tag{25.6.7}$$

where $C\beta^{-2}\bar{r}\Theta$ estimates the last term in the right-hand expression of (25.5.36). Then

$$\begin{aligned}\mathsf{I}_N \int \ell(x)\rho_\Psi(x)\theta(x)\,dx \le \int \theta(x)V(x)\ell(x)\rho_\Psi(x)\,dx\\ - \int \Bigl(\rho^{(2)}_\Psi(x,y) - \rho_\Psi(x)\rho(y)\Bigr)\ell(x)|x-y|^{-1}\theta(x)\,dxdy\\ - \int \rho_\Psi(x)\rho(y)\ell(x)|x-y|^{-1}\theta(x)\,dxdy + C\beta^{-2}\bar{r}\Theta.\end{aligned} \tag{25.6.8}$$

Let us estimate from above

$$\begin{aligned}- \int \Bigl(\rho^{(2)}_\Psi(x,y) - \rho_\Psi(x)\rho(y)\Bigr)\ell(x)|x-y|^{-1}\theta(x)\,dxdy \le\\ - \int \Bigl(\rho^{(2)}_\Psi(x,y) - \rho_\Psi(x)\rho(y)\Bigr)\bigl(1-\omega(x,y)\bigr)\ell(x)|x-y|^{-1}\theta(x)\,dxdy\\ + \int \rho_\Psi(x)\rho(y)\omega(x,y)\ell(x)|x-y|^{-1}\theta(x)\,dxdy\end{aligned} \tag{25.6.9}$$

with $\omega = \omega_\gamma$: $\omega = 0$ for $|x-y| \ge 2\gamma$ and $\omega = 1$ for $|x-y| \le \gamma$, $\gamma \ge \beta$.

To estimate the first term in the right-hand expression one can apply Proposition 25.5.1. In this case $\|\nabla_y\chi\|_{\mathscr{L}^2}\asymp C\bar{r}\gamma^{-\frac{1}{2}}$, $\|\nabla_y\chi\|_{\mathscr{L}^\infty}\asymp \bar{r}\gamma^{-2}$ and plugging $P=\beta^{-2}\Theta$ and $T=|\nu|$, $\varepsilon=Z^{-\frac{2}{3}}$ we conclude that this term does not exceed

$$C\bar{r}\bigl(\gamma^{-\frac{1}{2}}\bar{Q}^{\frac{1}{2}}+CZ^{\frac{2}{3}}\gamma^{-2}\bigr)\Theta,\qquad \bar{Q}=\max(Q,Z^{\frac{5}{3}}).\tag{25.6.10}$$

Consider the second term in the right-hand expression of (25.6.9). Note that

$$\int \rho(y)\omega(x,y)|x-y|^{-1}\,dy\le C(\bar{r}^{-\frac{15}{2}}\gamma^{\frac{7}{2}}+\upsilon^{\frac{3}{2}}\gamma^2)$$

since $\rho(y)\asymp \bigl(W(y)+\nu\bigr)^{\frac{3}{2}}$ and $|\nabla W|\asymp \bar{r}^{-5}$; then this term does not exceed $C(\bar{r}^{-\frac{15}{2}}\gamma^{\frac{7}{2}}+\upsilon^{\frac{3}{2}}\gamma^2)\bar{r}\Theta$.

Adding to (25.6.10) we get

$$C\Bigl(\gamma^{-\frac{1}{2}}\bar{Q}^{\frac{1}{2}}+CZ^{\frac{2}{3}}\gamma^{-2}+\bar{r}^{-\frac{15}{2}}\gamma^{\frac{7}{2}}+\upsilon^{\frac{3}{2}}\gamma^2\Bigr)\bar{r}\Theta.$$

Optimizing with respect to $\gamma=\bar{Q}^{\frac{1}{5}}\upsilon^{-\frac{3}{5}}$ we get $C\upsilon^{\frac{3}{10}}\bar{Q}^{\frac{2}{5}}\bar{r}\Theta$ and (25.6.8) becomes

$$\begin{aligned}(\mathsf{I}_N+\nu)\int \ell(x)\rho_\Psi(x)\theta(x)\,dx\le\\ \int\theta(x)\bigl(W(x)+\nu\bigr)\ell(x)\rho_\Psi(x)\,dx+C\upsilon^{\frac{3}{10}}Q^{\frac{2}{5}}\bar{r}\Theta\le\\ C\bigl(\upsilon+\upsilon^{\frac{3}{10}}\bar{Q}^{\frac{2}{5}}\bigr)\bar{r}\Theta.\end{aligned}\tag{25.6.11}$$

where we took into account that $V-|x|^{-1}*\rho=W$, and that $W+\nu\le\upsilon$ on $\mathsf{supp}(\theta)$.

Since a factor at $(\mathsf{I}_N+\nu)$ in the left-hand expression of (25.6.11) is obviously $\asymp\bar{r}\Theta$ we arrive to $(\mathsf{I}_N+\nu)\le C\upsilon+\upsilon^{\frac{3}{10}}\bar{Q}^{\frac{2}{5}}$.

Recalling definition (25.6.4) of υ we arrive to an upper estimate in Theorem 25.6.3 below:

$$\mathsf{I}_N+\nu\le C\upsilon=CQ^{\frac{1}{6}}(Z-N)^{\frac{17}{18}}.\tag{25.6.12}$$

Really, this is true if $Q\ge Z^{\frac{5}{3}}$ (we are interested in the general approach) and in this case $\upsilon\ge\upsilon^{\frac{3}{10}}Q^{\frac{2}{5}}$. On the other hand, if $Q=Z^{\frac{5}{3}}(aZ^{\frac{1}{3}})^{-\delta}$, $aZ^{\frac{1}{3}}\ge 1$, then we get an extra term $CQ^{\frac{1}{20}}(Z-N)^{\frac{1}{5}}Z^{\frac{2}{3}}$ but we can skip it decreasing unspecified exponent $\delta>0$ in the definition of Q.

Remark 25.6.1. (i) We will prove the same estimate from below in the next Subsection 25.6.2.

(ii) Note that the relative error in the estimates is $\upsilon/\nu = (Z-N)^{-\frac{7}{2}}Q^{\frac{1}{6}}$.

(iii) In the proof we used not assumption (25.6.2) itself but its corollary (25.6.3). If we do not have such assumption instead of equality (25.6.4) we have inequality $\Theta^{\mathsf{TF}} \gtrsim \upsilon^{\frac{5}{2}}\bar{r}^7$ (but probably equality still holds). However we have a problem to estimate $|\Theta - \Theta^{\mathsf{TF}}|$: namely, we need to estimate the first factor in the product $\|\nabla\theta^{\frac{1}{2}}\|\mathsf{D}(\rho-\rho^{\mathsf{TF}},\rho-\rho^{\mathsf{TF}})^{\frac{1}{2}}$.

Let us select f in (25.6.1) such that $|f'|\le cf^{1-\delta/2}$ with arbitrarily small $\delta>0$. Then

$$b^2\|\nabla\theta^{\frac{1}{2}}\|^2 \le C\int_{\mathcal{Z}}\theta^{1-\delta}\,dx \le C(\int_{\mathcal{Z}}\theta\,dx)^{1-\delta}C(\int_{\mathcal{Z}}1\,dx)^{\delta}\le C(\Theta^{\mathsf{TF}})^{1-\delta}\upsilon^{-\frac{3}{2}(1-\delta)}\bar{r}^{3\delta}$$

with $\mathcal{Z}=\mathsf{supp}(\nabla\theta)$ and $\beta=\bar{r}^{\frac{13}{6}}Q^{\frac{1}{6}}$ and an error is less than $\epsilon\Theta^{\mathsf{TF}}$ provided

$$\upsilon = C_2\bar{r}^{-\frac{17}{6}}Q^{\frac{1}{6}}\times(\bar{r}^7Q)^{-\delta_1}$$

which leads to a marginally larger error.

Estimate P could be done in the same manner but here slight increase of it does not matter.

(iv) The same arguments of (iii) could be applied to the proof of the lower estimate in the next subsection despite rather different definition of Θ_Ψ by (25.6.18).

(v) In vrirtue of Theorem 25.6.4 stable molecules do not exist in the free nuclei model as $Z-N\ge CQ^{\frac{3}{7}}$ and in atomic case $\widehat{\mathsf{I}}_N=\mathsf{I}_N$.

Problem 25.6.2. Consider f such that $|f'|\le fg(f)$ where $g^{-1}(t)\in\mathscr{L}^1$ and further improve remainder estimate without assumption (25.6.3).

25.6.2 Estimate from below for Ionization Energy

Now let us prove estimate $\mathsf{I}_N+\nu$ from below. Let $\Psi=\Psi_N(x_1,\dots,x_N)$ be the ground state for N electrons, $\|\Psi\|=1$; consider an antisymmetric test function

$$\tilde{\Psi} = \tilde{\Psi}(x_1, \dots, x_{N+1}) = \Psi(x_1, \dots, x_N)u(x_{n+1}) - \sum_{1\le j\le N} \Psi(x_1, \dots, x_{j-1}, x_{N+1}, x_{j+1}, \dots, x_N)u(x_j). \tag{25.6.13}$$

Then

$$\begin{aligned}
&\mathsf{E}_{N+1}\|\tilde{\Psi}\|^2 \le \langle \mathsf{H}_{N+1}\tilde{\Psi}, \tilde{\Psi}\rangle = N\langle \mathsf{H}_{N+1}\Psi u, \tilde{\Psi}\rangle = \\
&\quad N\langle \mathsf{H}_N \Psi u, \tilde{\Psi}\rangle + N\langle H_{V, x_{N+1}}\Psi u, \tilde{\Psi}\rangle + N\langle \sum_{1\le i\le N} |x_i - x_{N+1}|^{-1}\Psi u, \tilde{\Psi}\rangle = \\
&\quad (\mathsf{E}_N - \nu')\|\tilde{\Psi}\|^2 + N\langle H_{W+\nu', x_{N+1}}\Psi u, \tilde{\Psi}\rangle \\
&\qquad + N\langle \big(\sum_{1\le i\le N} |x_i - x_{N+1}|^{-1} - (V - W)(x_{N+1})\big)\Psi u, \tilde{\Psi}\rangle
\end{aligned}$$

and therefore

$$\begin{aligned}
N^{-1}(\mathsf{I}_{N+1} + \nu')\|\tilde{\Psi}\|^2 \ge &-\langle H_{W+\nu', x_{N+1}}\Psi u, \tilde{\Psi}\rangle \\
&- \langle \big(\sum_{1\le i\le N} |x_i - x_{N+1}|^{-1} - (V - W)(x_{N+1})\big)\Psi u, \tilde{\Psi}\rangle
\end{aligned} \tag{25.6.14}$$

with $\nu' \ge \nu$ to be chosen later. One can see easily that

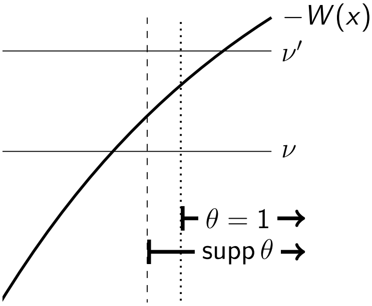
$$\begin{aligned}
N^{-1}\|\tilde{\Psi}\|^2 = \|\Psi\|^2 \cdot \|u\|^2 - \\
N\int \Psi(x_1, \dots, x_{N-1}, x)\Psi^\dagger(x_1, \dots, x_{N-1}, y)u(y)u^\dagger(x)\, dx_1 \cdots dx_{N-1}\, dxdy
\end{aligned} \tag{25.6.15}$$

where † means a complex or Hermitian conjugation.

Note that every term in the right-hand expression in (25.6.14) is the sum of two terms: one with $\tilde{\Psi}$ replaced by $\Psi(x_1, \dots, x_N)u(x_{N+1})$ and another with $\tilde{\Psi}$ replaced by $-N\Psi(x_1, \dots, x_{N-1}, x_{N+1})u(x_N)$. We call these terms *direct* and *indirect*indirect term respectively.

Obviously, in the direct and indirect terms u appears as $|u(x)|^2\, dx$ and as $u(x)u^\dagger(y)\, dxdy$ respectively, multiplied by some kernels.

Recall that u is an arbitrary function. Let us take $u(x) = \theta^{\frac{1}{2}}(x)\phi_j(x)$ where ϕ_j are orthonormal eigenfunctions of $H_{W+\nu}$ and $\theta(x)$ is β-admissible function supported in $\{x\colon -\upsilon \ge W(x)+\nu \ge \frac{2}{3}\nu\}$ and equal 1 in $\{x\colon | -2\upsilon \ge W(x)+\nu \ge \frac{1}{2}\nu\}$, satisfying (25.5.11), and $\beta = \upsilon\bar{r}^5$.



Let us substitute it into (25.6.14), multiply by $\varphi(\lambda_j L^{-1})$ and take sum with respect to j. We get the same expressions with $|u(x)|^2\,dx$ and $u(x)u^\dagger(y)\,dxdy$ replaced by $F(x,x)\,dx$ and $F(x,y)\,dxdy$ respectively with

$$F(x,y) = \int \varphi(\lambda L^{-1})\, d_\lambda e(x,y,\lambda). \tag{25.6.16}$$

Here $\varphi(\tau)$ is a fixed $\mathscr{C}^\infty$ non-negative function equal to 1 as $\tau \le \frac{1}{2}$ and equal to 0 as $\tau \ge 1$ and $L = \nu' - \nu = 6\upsilon$.

Under described construction and procedures the direct term generated by $N^{-1}\|\tilde{\Psi}\|^2$ is

$$\int \theta(x)\varphi(\lambda L^{-1})\, d_\lambda e(x,x,\lambda)\, dx \tag{25.6.17}$$

and applying the semiclassical approximation we get

$$\Theta_\Psi := \int \varphi(\lambda L^{-1})\, d_\lambda P'(W+\nu-\lambda)\, dx. \tag{25.6.18}$$

Therefore under assumptions (25.3.33) and (25.6.2)[24] the remainder estimate is $C\hbar^{-1}\bar{r}^2 b^{-2} = C\upsilon^{\frac{1}{2}}\bar{r}^2 b^{-1} = C\upsilon^{-\frac{1}{2}}\bar{r}^{-3}$; one can prove it easily by partition of unity on $\mathsf{supp}(\theta)$ and applying the semiclassical asymptotics with effective semiclassical parameter $\hbar = 1/(\upsilon^{\frac{1}{2}} b) = \upsilon^{-\frac{3}{2}}\bar{r}^{-5}$.

On the other hand, indirect term generated by $N^{-1}\|\tilde{\Psi}\|^2$ is

$$-N\int \theta^{\frac{1}{2}}(x)\theta^{\frac{1}{2}}(y)\Psi(x_1,\dots,x_{N-1},x)\Psi^\dagger(x_1,\dots,x_{N-1},y)\times F(x,y)\, dxdydx_1\cdots dx_{N-1} \tag{25.6.19}$$

[24] Or rather its corollary (25.6.3).

and since the operator norm of $F(.,.,.)$ is 1 the absolute value of this term does not exceed

$$N\int \theta(x)|\Psi(x_1,\dots,x_{N-1},x)|^2\,dx = \int \theta(x)\rho_\Psi(x)\,dx \le \int \theta(x)\rho(x)\,dx + CQ^{\frac{1}{2}}\|\nabla\theta^{\frac{1}{2}}\| \tag{25.6.20}$$

where $\rho^{\mathsf{TF}} = 0$ on $\operatorname{supp}(\theta)$ and under assumption (25.6.2)[24] $\|\nabla\theta^{\frac{1}{2}}\| \asymp b^{-\frac{1}{2}}\bar{r} \asymp \zeta^{-\frac{1}{2}}\bar{r}^{-\frac{3}{2}}$.

Recall that $P'(W^{\mathsf{TF}}+\nu)=\rho^{\mathsf{TF}}$. We will take $\nu'=\nu+L$ large enough to keep Θ_Ψ larger than all the remainders including those due to replacement W by W^{TF} and ρ by ρ^{TF} in the expression above. One can see easily that

$$\Theta_\Psi \asymp \hbar^{-3}\times b^{-2}\bar{r}^2 \asymp \upsilon^{\frac{3}{2}} b\bar{r}^2 \asymp \upsilon^{\frac{5}{2}}\bar{r}^7. \tag{25.6.21}$$

Therefore

(25.6.22) If $\upsilon = C_0\bar{r}^{-\frac{17}{6}}Q^{\frac{1}{6}}$ and $Z-N\ge C_0 Z^{\frac{5}{7}}$ the total expression generated by $N^{-1}\|\tilde{\Psi}\|^2$ is greater than $\epsilon\Theta$ with $\Theta=\upsilon^{\frac{5}{2}}\bar{r}^7$.

Now let us consider direct terms in the right-hand expression of (25.6.14). The first of them is

$$\begin{gathered}
-\int \theta^{\frac{1}{2}}(x)\varphi(\lambda L^{-1})\,d_\lambda\bigl(H_{W+\nu',x}\theta^{\frac{1}{2}}(x)e(x,y,\lambda)\bigr)_{y=x}\,dx = \\
-\int \theta(x)\varphi(\lambda L^{-1})\,d_\lambda\bigl(H_{W+\nu',x}e(x,y,\lambda)\bigr)_{y=x}\,dx \\
-\frac{1}{2}\int \varphi(\lambda L^{-1})[[H_W,\theta^{\frac{1}{2}}],\theta^{\frac{1}{2}}]\,d_\lambda e(x,x,\lambda) \ge \\
\int \theta(x)(\nu'-\nu-\lambda)\varphi(\lambda L^{-1})\,d_\lambda e(x,x,\lambda)\,dx - C\int |\nabla\theta^{\frac{1}{2}}|^2 e(x,x,\nu')dx.
\end{gathered} \tag{25.6.23}$$

Note that the absolute value of last term in the right-hand expression of (25.6.23) does not exceed $Cb^{-1}\bar{r}^2L^{\frac{3}{2}} \asymp C\upsilon^{\frac{1}{2}}\bar{r}^{-3} \ll C\upsilon\Theta$.

The second direct term in the right-hand expression is

$$\begin{gathered}
-\int \theta(x)\Bigl(\rho_\Psi * |x|^{-1} - (V-W)(x)\Bigr)F(x,x)\,dx = \\
-\mathsf{D}\bigl(\rho_\Psi-\bar{\rho},\theta(x)F(x,x)\bigr) \ge \\
-C\mathsf{D}\bigl(\rho_\Psi-\rho,\rho_\Psi-\rho\bigr)^{\frac{1}{2}}\cdot \mathsf{D}\Bigl(\theta^{\frac{1}{2}}F(x,x),\theta^{\frac{1}{2}}F(x,x)\Bigr)^{\frac{1}{2}} \ge -CQ^{\frac{1}{2}}\bar{r}^{\frac{15}{2}}\upsilon^{\frac{5}{2}}
\end{gathered} \tag{25.6.24}$$

provided $V-W=|x|^{-1}*\rho$ with $\mathsf{D}(\rho-\rho^{\mathsf{TF}},\rho-\rho^{\mathsf{TF}})\le CQ$; the absolute value of this term is $\ll \upsilon\Theta$.

Further, the first indirect term in the right-hand expression of (25.6.14) is

$$\begin{aligned}(25.6.25)\quad &-N\int \theta^{\frac{1}{2}}(y)\Psi(x_1,\dots,x_{N-1},x)\Psi^\dagger(x_1,\dots,x_{N-1},y)\times\\ &\qquad\varphi(\lambda L^{-1})\,d_\lambda\bigl(H_{W+\nu',x}\theta^{\frac{1}{2}}(x)e(x,y,\lambda)\bigr)\,dxdydx_1\cdots dx_{N-1}=\\ &-N\int \theta^{\frac{1}{2}}(y)\theta^{\frac{1}{2}}(x)\Psi(x_1,\dots,x_{N-1},x)\Psi^\dagger(x_1,\dots,x_{N-1},y)\times\\ &\qquad\varphi(\lambda L^{-1})(\nu'-\nu-\lambda)\,d_\lambda e(x,y,\lambda)\,dxdydx_1\cdots dx_{N-1}\\ &-N\int \theta^{\frac{1}{2}}(y)\Psi(x_1,\dots,x_{N-1},x)\Psi^\dagger(x_1,\dots,x_{N-1},y)\times\\ &\qquad\varphi(\lambda L^{-1})[H_{W,x},\theta^{\frac{1}{2}}(x)]\,d_\lambda e(x,y,\lambda)\,dxdydx_1\cdots dx_{N-1}.\end{aligned}$$

Note that one can rewrite the sum of the first terms in the right-hand expressions in (25.6.23) and (25.6.25) as $\sum_j \varphi(\lambda_j L^{-1})(\nu'-\nu-\lambda_j)\|\hat{\Psi}_j\|^2$ with

$$\hat{\Psi}_j(x_1,\dots,x_{N-1}):=\int \Psi(x_1,\dots,x_{N-1},x)\theta^{\frac{1}{2}}(x)\phi_j(x)\,dx$$

and therefore this sum is non-negative.

One can prove easily that the absolute value of the second term in (25.6.25) is less than

$$C\upsilon^{\frac{1}{2}}b^{-1}\int \rho_\Psi(y)\theta^{\frac{1}{2}}(y)\,dy\le C\upsilon^{-\frac{1}{2}}\bar{r}^{-5}\Theta\ll\upsilon\Theta.$$

Therefore

(25.6.26) The sum of the first direct and indirect terms in the right-hand expression of (25.6.14) is greater than $-C\upsilon\Theta$.

Finally, we need to consider the second indirect term generated by the right-hand expression of (25.6.14)

$$\begin{aligned}(25.6.27)\quad &-\int\Bigl(\sum_{1\le i\le N}|y-x_i|^{-1}-(V-W)(y)\Bigr)\times\\ &\Psi(x_1,\dots,x_N)\Psi^\dagger(x_1,\dots,x_{N-1},y)\theta^{\frac{1}{2}}(x_N)\theta^{\frac{1}{2}}(y)F(x_N,y)\,dx_1\cdots dx_N dy=\end{aligned}$$

$$-\int \Bigl(|y|^{-1}*\rho_{\underline{x}}(y)-(V-W)(y)\Bigr)\Psi(x_1,\dots,x_N)\Psi^\dagger(x_1,\dots,x_{N-1},y)\times \\ \theta^{\frac12}(x_N)\theta^{\frac12}(y)F(x_N,y)\,dx_1\cdots dx_N dy$$

$$-\int\Bigl(\sum_{1\le i\le N}|y-x_i|^{-1}-|y|^{-1}*\rho_{\underline{x}}(y)\Bigr)\Psi(x_1,\dots,x_N)\Psi^\dagger(x_1,\dots,x_{N-1},y)\times \\ \theta^{\frac12}(x_N)\theta^{\frac12}(y)F(x_N,y)\,dx_1\cdots\,dx_N dy;$$

recall that $\rho_{\underline{x}}$ is a smeared density, $\underline{x}=(x_1,\dots,x_N)$.

Since $|y|^{-1}*\rho_{\underline{x}}(y)-(V-W)(y)=|y|^{-1}*(\rho_{\underline{x}}-\rho)$, the first term in the right-hand expression is equal to

$$\int \theta^{\frac12}(x_N)\Psi(x_1,\dots,x_N)\times \\ \mathsf{D}_y\Bigl(\rho_{\underline{x}}(y)-\rho(y),F(x_N,y,\lambda)\theta^{\frac12}(y)\Psi(x_1,\dots,x_{N-1},y)\Bigr)\,dx_1\cdots dx_N; \tag{25.6.28}$$

and its absolute value does not exceed

$$\Bigl(N\int \mathsf{D}\bigl(\rho_{\underline{x}}(\cdot)-\rho(\cdot),\rho_{\underline{x}}(\cdot)-\rho(\cdot)\bigr)|\Psi(x_1,\dots,x_N)|^2\theta(x_N)\,dx_1\cdots dx_N\Bigr)^{\frac12}\times \\ N^{-\frac12}\Bigl(\mathsf{D}_y\Bigl(F(x_N,y,\lambda)\theta^{\frac12}(y)\Psi(x_1,\dots,x_{N-1},y), \\ F(x_N,y,\lambda)\theta^{\frac12}(y)\Psi(x_1,\dots,x_{N-1},y)\Bigr)\,dx_1\cdots dx_N\Bigr)^{\frac12}. \tag{25.6.29}$$

Due to estimate (25.5.24) and definition (25.5.4) as the first factor in (25.6.29) does not exceed $\bigl((Q+T+\varepsilon^{-1}N)\Theta+P\bigr)^{\frac12}$ where we assume that $\varepsilon\le Z^{-\frac23}$ and $\Theta\asymp b^{-\frac12}Q^{\frac12}\bar{r}$ is now an upper estimate for $\int\theta(y)\rho_\Psi(y)\,dy$-like expressions; due to our choice of υ it coincides with $\Theta=\upsilon^{\frac52}\bar{r}^7$.

Then according to (25.5.25) $P\asymp Cb^{-2}\Theta\ll Q\Theta$ and according to (25.5.23) $T\ll Q$ and therefore in all such inequalities we may skip P and T terms; so we get $C(Q+\varepsilon^{-1}N)^{\frac12}\Theta^{\frac12}$.

Meanwhile the second factor in (25.6.29) (without square root) is equal to

$$N^{-1}\int L^{-2}\varphi'(\lambda L^{-1})\varphi'(\lambda' L^{-1})|y-z|^{-1}\,\underbracket{e(x_N,y,\lambda)}\,\theta^{\frac{1}{2}}(y)\Psi(x_1,\ldots,x_{N-1},y)\times\\
\underbracket{e(x_N,z,\lambda')}\,\theta^{\frac{1}{2}}(z)\Psi^\dagger(x_1,\ldots,x_{N-1},z)\,dydz\,dx_1\cdots dx_{N-1}\,\underbracket{dx_N}\,d\lambda d\lambda';$$

after integration by x_N we get instead of marked terms $e(y,z,\lambda)$ (recall that $e(.,.,.)$ is the Schwartz kernel of projector and we keep $\lambda<\lambda'$) and then integrating with respect to λ' we arrive to

$$N^{-1}\int |y-z|^{-1}F(y,z)\theta^{\frac{1}{2}}(y)\Psi(x_1,\ldots,x_{N-1},y)\times\\
\theta^{\frac{1}{2}}(z)\Psi^\dagger(x_1,\ldots,x_{N-1},z)\,dydz\,dx_1\cdots dx_{N-1}$$

where now F is defined by (25.6.16) albeit with φ^2 instead of φ. This latter expression does not exceed

$$N^{-1}\iint |y-z|^{-1}|F(y,z)|\theta^{\frac{1}{2}}(y)|\Psi(x_1,\ldots,x_{N-1},y)|^2\times\\
dydz\,dx_1\cdots dx_{N-1}. \tag{25.6.30}$$

Then due to proposition 25.A.3 expression $\int |y-z|^{-1}|F(y,z)|\,dz$ does not exceed $Cb^{-1}\hbar^{-1}\asymp \upsilon^{\frac{1}{2}}$, and thus expression (25.6.30) does not exceed $CZ^{-2}\upsilon^{\frac{1}{2}}\Theta$ and therefore the second factor in (25.6.29) does not exceed $CN^{-1}\upsilon^{\frac{1}{4}}\Theta^{\frac{1}{2}}$ and the whole expression (25.6.29) does not exceed

$$C(Q+\varepsilon^{-1}N)^{\frac{1}{2}}\Theta^{\frac{1}{2}}\times N^{-1}\upsilon^{\frac{1}{4}}\Theta^{\frac{1}{2}} = CN^{-1}(Q+\varepsilon^{-1}N)^{\frac{1}{2}}\upsilon^{\frac{1}{4}}\Theta$$

and then

(25.6.31) As $\varepsilon\ge Z^{-1}\upsilon^{-\frac{3}{2}}$ the first term in the right-hand expression of (25.6.27) does not exceed $C\upsilon\Theta$.

Further, we need to estimate the second term in the right-hand expression of (25.6.27). It can be rewritten in the form

$$\sum_{1\le i\le N}\int U(x_i,y)\Psi(x_1,\ldots,x_N)\Psi^\dagger(x_1,\ldots,x_{N-1},y)\theta^{\frac{1}{2}}(x_N)\theta^{\frac{1}{2}}(y)\times\\
F(x_N,y)\,dx_1\cdots dx_N dy \tag{25.6.32}$$

where $U(x_i, y)$ is the difference between potential generated by the charge $\delta(x - x_i)$ and the same charge smeared; note that $U(x_i, y)$ is supported in $\{(x_i, y)\colon |x_i - y| \le \varepsilon\}$. Let us estimate the i-th term in this sum with $i < N$ first; multiplied by $N(N-1)$, it does not exceed

(25.6.33)
$$N\Bigl(\int |U(x_i,y)|^2|\Psi(x_1,\ldots,x_N)|^2\theta^{\frac{1}{2}}(x_N)\theta^{\frac{1}{2}}(y)|F(x_N,y)|\,dx_1\cdots dx_N dy\Bigr)^{\frac{1}{2}}\times$$
$$N\Bigl(\int \omega(x_i,y)|\Psi(x_1,\ldots,x_{N-1},y)|^2\theta^{\frac{1}{2}}(x_N)\theta^{\frac{1}{2}}(y)|F(x_N,y)|\,dx_1\cdots dx_N dy\Bigr)^{\frac{1}{2}};$$

here ω is ε-admissible and supported in $\{(x_i, y)\colon |x_i - y| \le 2\varepsilon\}$ function. Due to Proposition 25.A.3 in the second factor $\int \theta^{\frac{1}{2}}(x_N)|F(x_N, y)|\,dx_N \le C$ and therefore the whole second factor does not exceed

$$C\Bigl(\underbrace{\int \theta^{\frac{1}{2}}(x)\omega(x,y)\rho^{(2)}_\Psi(x,y)\,dxdy}\Bigr)^{\frac{1}{2}} \tag{25.6.34}$$

where we replaced x_i by x. According to Proposition 25.5.1 in the selected expression one can replace $\varrho^{(2)}_\Psi(x, y)$ by $\rho_\Psi(x)\rho(y)$ with an error which does not exceed

$$C\Bigl(\sup_x \|\nabla_y\chi_x\|_{\mathscr{L}^2(\mathbb{R}^3)}\bigl(Q+\varepsilon^{-1}N\bigr)^{\frac{1}{2}} + C\varepsilon N\|\nabla_y\chi\|_{\mathscr{L}^\infty}\Bigr)\Theta$$

which as we plug $\sup_x \|\nabla_y\chi_x\|_{\mathscr{L}^2(\mathbb{R}^3)} \asymp \varepsilon^{\frac{1}{2}}$, $\|\nabla_y\chi\|_{\mathscr{L}^\infty} \asymp \varepsilon^{-1}$ becomes $CN\Theta$. Meanwhile, consider

$$\int |U(x_i,y)|^2\theta^{\frac{1}{2}}(y)|F(x_N,y)|\,dy. \tag{25.6.35}$$

Again due to Proposition 25.A.3 it does not exceed

$$C\upsilon^{\frac{3}{2}}\int |U(x_i,y)|^2\theta^{\frac{1}{2}}(y)\bigl(|x_N-y|\upsilon^{\frac{1}{2}}+1\bigr)^{-s}\,dy$$

and this integral should be taken over $B(x_i, \varepsilon)$, with $|U(x_i, y)| \le |x_i - y|^{-1}$, so (25.6.35) does not exceed $C\varepsilon\upsilon^{\frac{3}{2}}\omega'(x_i, x_N)$ with $\omega'(x, y) = \bigl(1 + \upsilon^{\frac{1}{2}}|x - y|\bigr)^{-s}$

(provided $\varepsilon \le \upsilon^{-\frac{1}{2}}$ which will be the case). Therefore the first factor in (25.6.33) does not exceed

$$C\varepsilon^{\frac{1}{2}}\upsilon^{\frac{3}{4}}\Bigl(\underbrace{\int \theta^{\frac{1}{2}}(x)\omega'(x,y)\rho^{(2)}_{\Psi}(x,y)\,dxdy}\Bigr)^{\frac{1}{2}}. \tag{25.6.36}$$

Therefore in selected expression one can replace $\rho^{(2)}_{\Psi}(x,y)$ by $\rho_{\Psi}(x)\rho(y)$ with an error which does not exceed what we got before but with ε replaced by $\upsilon^{-\frac{1}{2}}$, i.e. also $CN\Theta$.

However in both selected expressions replacing $\rho^{(2)}_{\Psi}(x,y)$ by $\rho_{\Psi}(x)\rho(y)$ we get just 0. Therefore expression (25.6.33) does not exceed $C\varepsilon^{\frac{1}{2}}\upsilon^{\frac{3}{4}}Z\Theta$ which does not exceed $C\upsilon\Theta$ provided $\varepsilon \le C\upsilon^{\frac{1}{2}}Z^{-2}$.

So, we have two restriction to ε from above: the last one and $\varepsilon \le Z^{-\frac{2}{3}}$ and one can see easily that both of them are compatible with with restriction to ε in (25.6.31).

Finally, consider term in (25.6.32) with $i=N$ (multiplied by N):

$$N\int U(x_N,y)|\Psi(x_1,\ldots,x_N)|^2\theta^{\frac{1}{2}}(x_N)\theta^{\frac{1}{2}}(y)F(x_N,y)\,dx_1\cdots dx_N dy; \tag{25.6.37}$$

due to Cauchy inequality it does not exceed

$$\begin{aligned} N\Bigl(\int |x_N-y|^{-2}|\Psi(x_1,\ldots,x_N)|^2\theta^{\frac{1}{2}}(x_N)\theta^{\frac{1}{2}}(y)\ dx_1\cdots dx_N dy\Bigr)^{\frac{1}{2}}\times\\ N\Bigl(\int |F(x_N,y)|^2|\Psi(x_1,\ldots,x_N)|^2\theta^{\frac{1}{2}}(x_N)\theta^{\frac{1}{2}}(y)\ dx_1\cdots dx_N dy\Bigr)^{\frac{1}{2}}\end{aligned} \tag{25.6.38}$$

where both integrals are taken over $\{|x_N-y|\le\varepsilon\}$ and integrating with respect to y there we get that it does not exceed

$$C\varepsilon^{\frac{1}{2}}\Theta^{\frac{1}{2}}\times\upsilon^{\frac{3}{4}}\varepsilon^{\frac{3}{2}}\Theta^{\frac{1}{2}} = C\upsilon^{\frac{3}{4}}\varepsilon^2\Theta \ll \upsilon\Theta.$$

Therefore the right-hand expression in (25.6.14) is $\ge -C\upsilon\Theta$ and recalling that $\nu'-\nu=O(\upsilon)$ we recover an lower estimate in Theorem 25.6.3 below:

$$\mathsf{I}_N+\nu \ge -C\upsilon = CQ^{\frac{1}{6}}(Z-N)^{\frac{17}{18}}. \tag{25.6.39}$$

Combining with a lower estimate (25.6.12) and recalling estimate (25.4.5) for Q we arrive to

Theorem 25.6.3. *Let condition* (25.3.33) *be fulfilled and let* $N\le Z-C_0Q^{\frac{3}{7}}$ *with* $Q\le C_1Z^{\frac{5}{3}}$.

Then in the framework of fixed nuclei model under assumption (25.6.2)

$$|\mathsf{I}_N+\nu|\le C(Z-N)^{\frac{17}{18}}Z^{\frac{5}{18}}\begin{cases}1 & \text{as}\quad a\le Z^{-\frac{1}{3}},\\ Z^{-\delta}+(aZ^{\frac{1}{3}})^{-\delta} & \text{as}\quad a\ge Z^{-\frac{1}{3}}.\end{cases}\tag{25.6.40}$$

25.6.3 Estimate for Excessive Positive Charge

To estimate excessive positive charge when molecules can still exist in free nuclei model we apply arguments of section 5 of B. Ruskai and J. P. Solovej [1]. In view of Theorem 25.4.15 it is sufficient to consider the case

$$a=\min_{j<k}|\mathsf{y}_j-\mathsf{y}_k|\ge C_0\bar{r}.\tag{25.6.41}$$

Therefore in Thomas-Fermi theory ρ^{TF} is supported in separate "atoms".

Let us consider a-admissible functions $\theta_m(x)$, supported in $B(\mathsf{y}_m,\frac{1}{3}a)$ for $m=1,\dots,M$ and in $\{|x-\mathsf{y}_m|\ge\frac{1}{4}a\ \forall m=1,\dots,M\}$ for $m=0$, such that

$$\theta_0^2+\dots+\theta_M^2=1.\tag{25.6.42}$$

Then for the ground state Ψ

$$\mathsf{E}_N=\langle\mathsf{H}\Psi,\Psi\rangle=\sum_\alpha\langle\theta_\alpha\mathsf{H}\theta_\alpha\Psi,\Psi\rangle-\sum_{\alpha,j}\|(\nabla_j\theta_\alpha)\Psi\|^2\tag{25.6.43}$$

with the sum over of $(M+1)$-cluster decompositions $\alpha=(\alpha_0,\dots,\alpha_M)$ of $\{1,\dots,N\}$ and $\theta_\alpha(\underline{x})=\prod_{0\le m\le M}\prod_{i\in\alpha_m}\theta_m(x_i)$; $j=1,\dots,N$. Then for any given α

$$\mathsf{H}=\sum_{0\le m\le M}\mathsf{H}_{\alpha_m}+J_\alpha\tag{25.6.44}$$

with the *cluster Hamiltonians* H_{α_m}, involving only potential of m-th nucleus (no nucleus potential as $m=0$) and only electrons belonging to α_m and therefore satisfying

$$\mathsf{H}_{\alpha_m}\ge\mathsf{E}_{\boldsymbol{at}}(N_m(\alpha),Z_m),\qquad\mathsf{H}_{\alpha_0}\ge0,\tag{25.6.45}$$

and with the *intercluster Hamiltonian* (actually, just potentials)

$$J_\alpha = \sum_{1\le m\le M}\sum_{i\notin\alpha_m} -Z_m|x_i-\mathsf{y}_m|^{-1} + \sum_{m<l}\sum_{i\in\alpha_m, j\in\alpha_l} |x_i-x_j|^{-1} + \sum_{m<l} Z_mZ_l|\mathsf{y}_l-\mathsf{y}_m|^{-1}. \tag{25.6.46}$$

Let us note that

$$\sum_\alpha \theta_\alpha^2 J_\alpha = \sum_{0\le m<l\le M} J_{ml} \tag{25.6.47}$$

with J_{ml} given by (32)–(33) of Ruskai–Solovej [1] if $m,l>0$ and $m=0$ respectively:

$$J_{ml} = Z_mZ_l|\mathsf{y}_m-\mathsf{y}_l|^{-1} - Z_m\sum_i \theta_l(x_i)^2|x_i-\mathsf{y}_m|^{-1} - Z_l\sum_i \theta_m(x_i)^2|x_i-\mathsf{y}_l|^{-1} + \sum_{i\ne j}\theta_m(x_i)^2\theta_l(x_j)^2|x_i-x_j|^{-1}, \tag{25.6.48}$$

and

$$J_{0l} = \sum_i \theta_0(x_i)^2\Bigl(-Z_l|x_i-\mathsf{y}_l|^{-1} + \sum_j \theta_l(x_j)^2|x_i-x_j|^{-1}\Bigr). \tag{25.6.49}$$

Then we recover (35) of Ruskai–Solovej [1]

$$\langle J_{ml}\Psi,\Psi\rangle = Z_mZ_l|\mathsf{y}_m-\mathsf{y}_l|^{-1} - Z_l\int \rho_\Psi(x)\theta_m(x)^2|x-\mathsf{y}_l|^{-1}\,dx - Z_m\int \rho_\Psi(x)\theta_l(x)^2|x-\mathsf{y}_m|^{-1}\,dx + \int \rho^{(2)}_\Psi(x,y)\theta_m(x)\theta_l(y)\,dxdy. \tag{25.6.50}$$

Applying Proposition 25.5.1 and estimate (25.4.56) (replacing first θ_m with $m=1,\dots,M$ by $\tilde\theta_m$ supported in $B(\mathsf{y}_m, c\bar r)$ and estimating an error), we conclude that

$$\int \rho_\Psi(x)\theta_m(x)^2|x-\mathsf{y}_l|^{-1}\,dx = \Bigl(\int \rho^{\mathsf{TF}}(x)\theta_m(x)^2|x-\mathsf{y}_l|^{-1}\,dx + O(Y)\Bigr)|\mathsf{y}_m-\mathsf{y}_l|^{-1}, \tag{25.6.51}$$

$$\int \rho_\Psi(x)\tilde\theta_m(x)^2\,dx = N_m^{\mathsf{TF}} + O(Y), \tag{25.6.52}$$

with

$$N_m^{\mathsf{TF}} = \int \rho^{\mathsf{TF}}(x)\theta_m(x)^2\,dx, \qquad Y := Q^{\frac12}\bar{r}^{\frac12} \tag{25.6.53}$$

(compare with (36)–(37) of Ruskai–Solovej [1]) which yields

$$\int \rho_\Psi(x)\bigl(1-\sum_{1\le m\le M}\tilde{\theta}_m(x)\bigr)\,dx \le CY, \tag{25.6.54}$$

and we prove that (25.6.52) holds for θ_m as well (compare with (38) of Ruskai–Solovej [1]).

The last term in (25.6.51) is estimated by Proposition 25.5.1 and estimate (25.4.56) and the same replacement trick:

$$\begin{aligned}\int \rho_\Psi^{(2)}(x,y)\theta_m(x)^2\theta_l(y)^2|x-y|^{-1}\,dxdy \ge\\ \int \rho_\Psi^{(2)}(x,y)\tilde{\theta}_m(x)^2\theta_l(y)^2|x-y|^{-1}\,dxdy \ge\\ \int \rho^{\mathsf{TF}}(x)\rho_\Psi(y)\tilde{\theta}_m(x)^2\theta_l(y)^2|x-y|^{-1}\,dxdy -\\ C\Bigl(Q^{\frac12}\int \rho_\Psi(x)\theta_l(x)^2dx + Ya^{-1}\Bigr)|\mathsf{y}_m-\mathsf{y}_l|^{-1}\end{aligned} \tag{25.6.55}$$

and repeating the same trick we get that it is larger than

$$\int \rho^{\mathsf{TF}}(x)\rho^{\mathsf{TF}}(y)|x-y|^{-1}dxdy - C(Z-N)Ya^{-1} - CY^2a^{-1}. \tag{25.6.56}$$

Then we conclude that

$$\langle J_{ml}\Psi,\Psi\rangle \ge J_{ml}^{\mathsf{TF}} - CNYa^{-1} \tag{25.6.57}$$

with

$$\begin{aligned}J_{ml}^{\mathsf{TF}} = \int \rho^{\mathsf{TF}}(x)\rho^{\mathsf{TF}}(y)\theta_m(x)\theta_l(y)|x-y|^{-1}\,dxdy\\ - Z_m\int \rho^{\mathsf{TF}}(x)\theta_l(y)|x-\mathsf{y}_m|^{-1}\,dx - Z_l\int \rho^{\mathsf{TF}}(x)\theta_m(y)|x-\mathsf{y}_l|^{-1}\,dx\\ + Z_mZ_l|\mathsf{y}_m-\mathsf{y}_l|^{-1}\end{aligned} \tag{25.6.58}$$

and

$$|\langle J_{0l}\Psi,\Psi\rangle| \le C(Z-N)Ya^{-1} + CY^2a^{-1} \tag{25.6.59}$$

(compare with (39)–(40) of Ruskai–Solovej [1]) provided

$$\Bigl|\int \rho^{\mathsf{TF}}(y)|x-y|^{-1}\tilde{\theta}_m(x)\,dy - N_m^{\mathsf{TF}}|x-\mathsf{y}_m|^{-1}\Bigr| \le C(Z-N)|x-\mathsf{y}_m|^{-1} \tag{25.6.60}$$

for $|x-\mathsf{y}_m|\ge C\bar{r}$.

Let us note that the absolute value of the last term in the right-hand expression of (25.6.43) does not exceed $Ca^{-2}Y$ due to (25.6.52). Now stability condition yields

$$J=\sum_{0\le m<l\le M} J_{ml}\le CYa^{-2}+C(Z-N)Ya^{-1}+CY^2a^{-1}. \tag{25.6.61}$$

This inequality, (25.6.41) and Proposition 25.6.6 below yield that $Z-N\le CY=C\bar{r}^{\frac{1}{2}}Q^{\frac{1}{2}}$. Since $\bar{r}\asymp (Z-N)^{-\frac{1}{3}}$ we arrive to $(Z-N)\le CQ^{\frac{3}{7}}$:

Theorem 25.6.4. *Let condition* (25.3.33) *be fulfilled. Then in the framework of free nuclei model with* $M\ge 2$ *the stable molecule does not exist unless*

$$Z-N\le Z^{\frac{5}{7}-\delta}. \tag{25.6.62}$$

Remark 25.6.5. Unfortunately, we do not prove that molecules exist. We are not aware of any rigorous result of this type in the frameworks of our models.

Proposition 25.6.6. *Let* (25.6.41) *be fulfilled. Then inequality* (25.6.60) *holds and*

$$J\ge \epsilon (Z-N)^2a^{-1}. \tag{25.6.63}$$

Proof. Note first that

$$\mathcal{E}^{\mathsf{TF}}\le \mathcal{E}(\bar{\rho})=\sum_j \mathcal{E}(\rho_j^{\mathsf{TF}})+J^{\mathsf{TF}}(\bar{\rho})\le \sum_j \mathcal{E}^{\mathsf{TF}}(\rho_j^{\mathsf{TF}})+C(Z-N)^2a^{-1} \tag{25.6.64}$$

with $\bar{\rho}=\sum_j\rho_j^{\mathsf{TF}}$ while

$$\sum_j \mathcal{E}(\rho_j^{\mathsf{TF}})\le \sum_j \mathcal{E}(\theta_j\rho^{\mathsf{TF}}); \tag{25.6.65}$$

then

$$J^{\mathsf{TF}}(\rho^{\mathsf{TF}}) \le C(Z-N)^2 a^{-1} \tag{25.6.66}$$

and using (25.6.62) we conclude that

$$\mathsf{D}(\rho^{\mathsf{TF}}-\bar\rho, \rho^{\mathsf{TF}}-\bar\rho) \le C(Z-N)^2 a^{-1}. \tag{25.6.67}$$

Further,

$$\Lambda := \sum_j \mathsf{D}(\rho^{\mathsf{TF}}\theta_j - \rho_j^{\mathsf{TF}}, \rho^{\mathsf{TF}}\theta_j - \rho_j^{\mathsf{TF}}) \le \\ \mathsf{D}(\rho^{\mathsf{TF}}-\bar\rho, \rho^{\mathsf{TF}}-\bar\rho) + C\bar r a^{-1}\Lambda \tag{25.6.68}$$

and combining with (25.6.66) we conclude that

$$\Lambda \le C(Z-N)^2 a^{-1} \tag{25.6.69}$$

due to (25.6.41). Combining with $\rho_j^{\mathsf{TF}} * |x|^{-1} = N_j^{\mathsf{TF}}|x-\mathsf{y}_j|^{-1}$ for $|x-\mathsf{y}_j| \ge r_S$ we arrive to (25.6.60). Further,

$$J^{\mathsf{TF}}(\rho^{\mathsf{TF}}) \ge J^{\mathsf{TF}}(\bar\rho) - C\Lambda^{\frac12}\bar r\frac{1}{2}(Z-N)a^{-\frac32} - C\Lambda\bar r^{-1} \tag{25.6.70}$$

which together with (25.6.68) and (25.6.69) yields (25.6.63). $\square$

25.A Appendices

25.A.1 Electrostatic Inequalities

We know already that there are two sources of errors in the lower estimate: due to electrostatic inequality (25.2.1) and semiclassical errors. For the first error in the case $\vec B = \mathsf{const}$ E. Lieb, J. P. Solovej and J. Yngvason [3] provide the (almost) perfect estimate; the reader can find the proof based on the magnetic Lieb–Thirring inequality (and this inequality as well) in that paper (p. 122) which in the case of $\vec B = 0$ becomes

Theorem 25.A.1. *For the ground state* Ψ *of* (25.1.1) *with potential* (25.1.4)

$$\int \rho_\Psi^{\frac43}\, dx \le CZ^{\frac56} N^{\frac12}(Z+N)^{\frac13} \tag{25.A.1}$$

otherwise.

In particular for $c^{-1}N \le Z \le cN$ *the right-hand expression does not exceed* $CZ^{\frac53}$*.*

On the other hand, for $B = 0$ there is a more precise inequality due to V. Bach [1] and G. Graf and J. P. Solovej [1]:

Theorem 25.A.2. *For the ground state* Ψ *of* (25.1.1) *with potential* (25.1.4)

$$\langle \mathsf{H}\Psi, \Psi\rangle \geq \mathsf{N}_1(A-\nu) + \nu N - \frac{1}{2}\iint |x-y|^{-1}|e(x,y,\nu)|^2\,dxdy - CN^{\frac{5}{3}-\delta} \tag{25.A.2}$$

with some exponent $\delta > 0$.

We will discuss magnetic field case in more details in the Appendix to the next Chapter 26.

25.A.2 Hamiltonian Trajectories

We are going to prove that for $W = W^{\mathsf{TF}}$ in $M = 1$ case the generic trajectory on the energy level ν is not periodic. We use some ideas from V. Arnold [2], pages 37–38. Recall that in this case $W = W(r)$ ($r = |x - \mathsf{y}_1|$) and angular momentum $\vec{M}$ is a motion integral. Then any trajectory lies on some plane and if $M = |\vec{M}| > 0$ it lies in $\{0 < r < \bar{r}\}$ where W is analytic and $W(\bar{r}) = -\nu$.

(25.A.3) Let us assume that all the trajectories on the energy level ν are periodic.

Then the rotation number

$$\Phi = \int_{r_1}^{r_2} \frac{M\,dr}{r^2\sqrt{2\bigl(W(r)+\nu\bigr) - M^2r^{-2}}} \tag{25.A.4}$$

showing the increment of the polar angle over a half-trajectory should be πk^{-1} with $k \in \mathbb{N}$ and should not depend on M where $r_1 \leq r_2$ are roots of $\bigl(W(r)+\nu\bigr) - M^2r^{-2} = \nu$. So, Φ should be the same for all trajectories on the energy level ν. One can see easily that for $M \to 0$ Φ tends to those of the Coulomb potential. So, $\Phi = 2\pi$ for all trajectories on the energy level ν.

Let r_0 be a root of $F(r) = 2\bigl(W(r)+\nu\bigr) + r^4\bigl(W'(r)\bigr)^2 = 0$. One can see easily that $F(\bar{r}) > 0$, $F(r) \to \infty$ as $r \to 0$ and $F'(r) < 0$ because

$$W' < 0, \qquad W'' + 2rW' = r^{-1}(r^2W')') = r\Delta W > 0. \tag{25.A.5}$$

So, the unique root exists. Then $r = r_0$ is a circular motion with $M = -r_0^3 W'(r_0)$.

Then (V. Arnold [2], problem 2 at page 37)

$$\Phi \to \pi\sqrt{W'/(3W' + rW'')^{-1}}\big|_{r=r_0} = \Phi_0$$

for trajectories tending to circular. However, $3W' + rW'' > W'$ due to (25.A.5) and then $\Phi_0 > \pi$. Contradiction to assumption (25.A.3).

25.A.3 Some Spectral Function Estimates

Proposition 25.A.3. *For Schrödinger operator with* $W \in \mathscr{C}^\infty$ *and for* $\phi \in \mathscr{C}_0^\infty([-1,1])$ *the following estimate holds for any* s*:*

$$|F(x,y)| \le Ch^{-3}\bigl(1 + h^{-1}|x-y|\bigr)^{-s}, \tag{25.A.6}$$

$$F(x,y) := \int \phi(\lambda)\, d_\lambda e(x,y,\lambda). \tag{25.A.7}$$

Proof. Let $u(x,y,t) = \int e^{-ih^{-1}t\lambda}\, d_\lambda e(x,y,\lambda)$ be the Schwartz's kernel of $e^{-ih^{-1}Ht}$.

Fix y. Note first that $\mathscr{L}^2$-norm[25)] of $\phi(hD_t)\chi(t)\omega(x)u(x,y,t)$ is less than Ch^s as $\chi \in \mathscr{C}_0^\infty([-\epsilon,\epsilon])$ and $\omega \in \mathscr{C}^\infty$ supported in $\{|x-y| \ge \epsilon_1\}$ ($\epsilon_1 = C\epsilon$) due to the finite speed of propagation of singularities.

We conclude then that $\mathscr{L}^2$-norm of $\phi(hD_t)\chi(t)\omega(x)u(x,y,t)$ is less than Ch^s for $\omega \in \mathscr{C}^\infty$ supported in $\{x\colon |x-y| \ge C\}$.

Then $\mathscr{L}^2$-norm of $\partial_t^l\nabla^\alpha\phi(hD_t)\chi(t)\omega(x)u$ does not exceed Ch^s. Then due to imbedding inequality $\mathscr{L}^\infty$-norm of $\phi(hD_t)\chi(t)\omega(x)u$ does not exceed Ch^s. Setting $t=0$ and using this inequality and $|F(x,y)| \le Ch^{-3}$ (due to Chapter 4) we get that $|F(x,y)| \le Ch^s$ for $|x-y| \ge \epsilon_0$;

Now let us consider general $|x-y| = r \ge Ch$. Rescaling $x-y \mapsto (x-y)r^{-1}$ we need to rescale $h \mapsto hr^{-1}$ and rescaling above inequality and keeping in mind that $F(x,y)$ is a density with respect to x we get $|F(x,y)| \le Ch^s r^{-3-s}$ which is equivalent to (25.A.6)–(25.A.7). □

Comments

There are papers of physicists. L.H. Thomas and E. Fermi have suggested in 1927 that a large Coulomb system (atom or molecule) in the ground

25) With respect to x, t here and below.

state looks like a classical gas but with the Pauli principle, so, leading to the first term $\mathcal{E}^{\mathsf{TF}}$ in the asymptotics. The second term of asymptotics was conjectured by J. M.C. Scott in 1952 as a contribution of those electrons which move very close to the nuclei. Next terms, Dirac and Schwinger corrections were conjectured in 1930 and 1980, respectively.

The mathematical rigorous papers one can separated into several groups:

First, there are papers concerning only the Thomas–Fermi model (so, studying the Thomas-Fermi equation, may be, with some modifications, without any consideration of the quantum mechanical model, even if the latter was a source for the former). Most notably H. Brezis, H. and E. Lieb E. [1], R. Benguria [1], R. Benguria, R. and Lieb E. H. [1].

The second group consists of the papers, justifying Thomas–Fermi model as an approximation to the quantum mechanical model: E. H. Lieb and B. Simon, [1], where the leading term was derived; also certain properties of the the Thomas–Fermi model were established.

Next, W. Hughes [1] and H. Siedentop and R. Weikart [1–3] justified the Scott correction term in the atomic case, while V. Ivrii and M. Sigal [1] justified it in the molecular case.

Then, C. Fefferman and L. Seco [1] justified Dirac and Schwinger correction terms in the atomic case, while V. Ivrii justified them in [21] (even in the case of the relatively weak magnetic field). J. P. Solovej, J. P., T. Ø. Sørensen and W. L. Spitzer [1] recovered Scott correction term in the relativistic case (under assumption preventing relativistic instability).

The third group consists of the papers, related to the ground state energy problem: B. Ruskai and J. P. Solovej [1], J. P. Solovej [1] and L. A. Seco, I. M. Sigal, and J. P. Solovej [1].

Finally, we already mentioned papers which provided the solid functional-analytical base for all this construction. Pretty complete survey could be found in C. L. Fefferman, V. Ivrii, L. A. Seco, and I. M. Sigal [1].

Chapter 26

The Case of External Magnetic Field

26.1 Introduction

In this Chapter we repeat analysis of the previous Chapter 25 but in the case of the constant external magnetic field[1)].

26.1.1 Framework

Let us consider the following operator (quantum Hamiltonian)

$$\mathsf{H} = \mathsf{H}_N := \sum_{1\le j\le N} H_{A,V,x_j} + \sum_{1\le j<k\le N} |x_j - x_k|^{-1} \tag{26.1.1}$$

on

$$\mathfrak{H} = \bigwedge_{1\le n\le N} \mathsf{H}, \qquad \mathsf{H} = \mathscr{L}^2(\mathbb{R}^d, \mathbb{C}^q) \tag{26.1.2}$$

with

$$H_{V,A} = \bigl((i\nabla - A)\cdot \boldsymbol{\sigma}\bigr)^2 - V(x) \tag{26.1.3}$$

describing N same type particles in the external field with the scalar potential $-V$ and vector potential $A(x)$, and repulsing one another according to the Coulomb law.

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1) Actually we need a magnetic field either sufficiently weak or close to a constant on the very small scale.

V. Ivrii, *Microlocal Analysis, Sharp Spectral Asymptotics and Applications V*, https://doi.org/10.1007/978-3-030-30561-1_26

Here $x_j \in \mathbb{R}^d$ and $(x_1, \dots, x_N) \in \mathbb{R}^{dN}$, potentials $V(x)$ and $A(x)$ are assumed to be real-valued. Except when specifically mentioned we assume that

$$V(x) = \sum_{1\le k\le M} \frac{Z_m}{|x - \mathsf{y}_m|} \tag{26.1.4}$$

where $Z_m > 0$ and y_m are charges and locations of nuclei. Here $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \dots, \sigma_d)$, σ_k are $q \times q$-Pauli matrices.

So far in comparison with the previous Chapter 25 we only changed (25.1.3) to (26.1.3) introducing magnetic field. Now spin enters not only in the definition of the space but also into operator through matrices σ_k. Since we need $d = 3$ Pauli matrices it is sufficient to consider $q = 2$ but we will consider more general case as well (but q should be even).

Remark 26.1.1. In the case of the the constant magnetic field $\nabla \times A$

$$H_{A,V} = \bigl(-i\nabla - A(x)\bigr)^2 + \boldsymbol{\sigma}\cdot(\nabla \times A) - V(x) \tag{26.1.5}$$

In the case $d = 2$ this operator downgrades to

$$H_{A,V} = \bigl(-i\nabla - A(x)\bigr)^2 + \sigma_3(\nabla \times A) - V(x) \tag{26.1.6}$$

Again, let us assume that

(26.1.7) Operator H is self-adjoint on $\mathfrak{H}$.

As usual we will never discuss this assumption.

26.1.2 Problems to Consider

As in the previous Chapter we are interested in the *ground state energy* $\mathsf{E} = \mathsf{E}_N$ of our system i.e. in the lowest eigenvalue of the operator $\mathsf{H} = \mathsf{H}_N$ on $\mathfrak{H}$:

$$\mathsf{E} := \inf \operatorname{Spec} \mathsf{H} \qquad \text{on } \ \mathfrak{H}; \tag{26.1.8}$$

more precisely, we are interested in the asymptotics of $\mathsf{E}_N = \mathsf{E}(\underline{\mathsf{y}}; \underline{Z}; N)$ as V is defined by (26.1.4) and $N \asymp Z := Z_1 + Z_2 + \ldots + Z_M \to \infty$ and we are going to prove that[2] E is equal to *Magnetic Thomas-Fermi energy* $\mathcal{E}_B^{\mathsf{TF}}$, possibly with the Scott and Dirac-Schwinger corrections and with an appropriate error.

We are also interested in the asymptotics for the *ionization energy*

$$\mathsf{I}_N := \mathsf{E}_{N-1} - \mathsf{E}_N \tag{26.1.9}$$

and we also would like to estimate *maximal excessive negative charge*

$$\max_{N\colon \mathsf{I}_N>0} (N - Z). \tag{26.1.10}$$

All these questions so far were considered in the framework of the fixed positions $\mathsf{y}_1, \dots, \mathsf{y}_M$ but we can also consider

$$\widehat{\mathsf{E}} := \widehat{\mathsf{E}}_N = \widehat{\mathsf{E}}(\underline{\mathsf{y}}; \underline{Z}; N) = \mathsf{E} + U(\underline{\mathsf{y}}; \underline{Z}) \tag{26.1.11}$$

with

$$U(\underline{\mathsf{y}}; \underline{Z}) := \sum_{1\le m<m'\le M} \frac{Z_m Z_{m'}}{|\mathsf{y}_m - \mathsf{y}_{m'}|} \tag{26.1.12}$$

and

$$\widehat{\mathsf{E}}(\underline{Z}; N) = \inf_{\mathsf{y}_1,\dots,\mathsf{y}_M} \widehat{\mathsf{E}}(\underline{\mathsf{y}}; \underline{Z}; N) \tag{26.1.13}$$

and replace I_N by $\widehat{I}_N = \widehat{\mathsf{E}}_{N-1} - \widehat{\mathsf{E}}_N$ and modify all our questions accordingly. We call these frameworks *fixed nuclei model* and *free nuclei model* respectively.

In the free nuclei model we can consider two other problems:

(a) Estimate from below *minimal distance between nuclei* i.e.

$$\min_{1\le m<m'\le M} |\mathsf{y}_m - \mathsf{y}_{m'}|$$

for which such minimum is achieved.

(b) Estimate *maximal excessive positive charge*

$$\max_N \bigl\{(Z - N)\colon \widehat{\mathsf{E}} < \min_{\substack{N_1,\dots,N_M\colon\\ N_1+\dots N_M=N}} \sum_{1\le m\le M} \mathsf{E}(Z_m; N_m)\bigr\} \tag{26.1.14}$$

for which molecule does not disintegrates into atoms.

[2] Under reasonable assumption to the minimal distance between nuclei.

26.1.3 Magnetic Thomas-Fermi Theory

As in the previous Chapter 25 the first approximation is the Hartree-Fock (or Thomas-Fermi) theory. Let us introduce the *spacial density* of the particle with the state $\Psi \in \mathfrak{H}$:

$$\rho(x) = \rho_\Psi(x) = N \int |\Psi(x, x_2, \dots, x_N)|^2 \, dx_2 \cdots dx_N. \tag{26.1.15}$$

Let us write the Hamiltonian, describing the corresponding "quantum liquid":

$$\mathcal{E}_B(\rho) = \int \tau_B(\rho(x))\, dx - \int V(x)\rho(x)\, dx + \frac{1}{2}\mathsf{D}(\rho, \rho), \tag{26.1.16}$$

with

$$\mathsf{D}(\rho,\rho) = \iint |x-y|^{-1}\rho(x)\rho(y)\, dxdy \tag{26.1.17}$$

where τ_B is the energy density of a gas of noninteracting electrons:

$$\tau_B(\rho) = \sup_{w\ge 0}\bigl(\rho w - P_B(w)\bigr) \tag{26.1.18}$$

is the Legendre transform of the *pressure* $P_B(w)$ given by the formula

$$P_B(w) = \varkappa_1 B\Bigl(\frac{1}{2} w_+^{\frac{d}{2}} + \sum_{j\ge 1} (w - 2jB)_+^{\frac{d}{2}}\Bigr) \tag{26.1.19}$$

with $\varkappa_1 = (2\pi)^{-1}q, (3\pi^2)^{-1}q$ for $d = 2, 3$ respectively.

The classical sense of the second and the third terms in the right-hand expression of (26.1.16) is clear and the density of the kinetic energy is given by $\tau_B(\rho)$ in the semiclassical approximation (see remark 26.1.2). So, the problem is

(26.1.20) Minimize functional $\mathcal{E}_B(\rho)$ defined by (26.1.16) under restrictions:

$$\rho \ge 0, \qquad \int \rho \, dx \le N. \tag{26.1.21$_{1,2}$}$$

The solution if exists is unique because functional $\mathcal{E}_B(\rho)$ is strictly convex (see below). The existence and the property of this solution denoted further by ρ_B^{TF} is known in the series of physically important cases.

Remark 26.1.2. If w is the negative potential then

$$\operatorname{tr} e(x,x,0) \approx P'_B(w) \tag{26.1.22}$$

defines the density of all non-interacting particles with negative energies at point x and

$$\int_{-\infty}^{0} \tau\, d_\tau \operatorname{tr} e(x,x,\tau)dx \approx -\int P_B(w)\, dx \tag{26.1.23}$$

is the total energy of these particles; here $\approx$ means "in the semiclassical approximation".

We consider in the case of $d=3$ a large (heavy) molecule with potential (25.1.4). It is well-known[3)] that

Proposition 26.1.3. *(i) For $V(x)$ given by* (26.1.4) *minimization problem* (26.1.20) *has a unique solution $\rho = \rho_B^{\mathsf{TF}}$; then denote $\mathcal{E}_B^{\mathsf{TF}} := \mathcal{E}_B(\rho_B^{\mathsf{TF}})$.*

(ii) Equality in $(26.1.21)_2$ *holds if and only if $N \le Z := \sum_m Z_m$.*

(iii) Further, ρ^{TF} does not depend on N as $N \ge Z$.

(iv) Thus

$$\int \rho_B^{\mathsf{TF}}\, dx = \min(N,Z), \qquad Z := \sum_{1\le m\le M} Z_m. \tag{26.1.24}$$

26.1.4 Main Results Sketched and Plan of the Chapter

In the first half of this Chapter we derive asymptotics for ground state energy and justify Thomas-Fermi theory. As construction of Section 25.2 works with minimal modifications (see Section 26.6) in the magnetic case as well we start immediately from magnetic Thomas-Fermi theory in Section 26.2.

We discover that there are three different cases: *a moderate magnetic field case $B \ll Z^{\frac{4}{3}}$* when $\mathcal{E}_B^{\mathsf{TF}} \asymp Z^{\frac{5}{3}}$ and $\mathcal{E}_B^{\mathsf{TF}} = \mathcal{E}_0^{\mathsf{TF}}(1+o(1))$, *a strong magnetic field case $B \gg Z^{\frac{4}{3}}$* when $\mathcal{E}_B^{\mathsf{TF}} \asymp B^{\frac{2}{5}} Z^{\frac{9}{5}}$ and $\mathcal{E}_B^{\mathsf{TF}} = \bar{\mathcal{E}}_B^{\mathsf{TF}}(1+o(1))$ where $\bar{\mathcal{E}}_B^{\mathsf{TF}}$

[3)] Section IV of E. H. Lieb, J. P. Solovej and J. Yngvason [3].

is Thomas-Fermi potential derived as $P_B(w) = \frac{1}{2}\varkappa_1 w^{\frac{d}{2}}$ (cf. (26.1.19)), and *an intermediate case* $B \sim Z^{\frac{4}{3}}$.

Then we apply semiclassical methods (like in Section 25.4) albeit now our analysis is way more complicated due to two factors: the semiclassical theory of the magnetic Schrödinger operator is more difficult than the corresponding theory for the non-magnetic Schrödinger operator and also Thomas-Fermi potential W^{TF} is not very smooth in the magnetic case, so we need to approximate it by a smooth one (on a microscale).

We discover that both semiclassical methods and Thomas-fermi theory are relevant only if $B \ll Z^3$. The case of the superstrong magnetic field $B \gg Z^3$ was considered in E. H. Lieb, J. P. Solovej and J. Yngvason [1].

First of all, in Section 26.3 we consider the case $M = 1$; then the Thomas-Fermi potential W_B^{TF} is non-degenerate and in this case we derive sharp spectral asymptotics.

Next, in Section 26.4 we consider the case $M \ge 2$ but we analyze only zone $\{W_B^{\mathsf{TF}} + \nu \gtrsim B\}$ where ν is a chemical potential and B is an intensity of the magnetic field. A certain weaker non-degeneracy condition is satisfied due to the Thomas-Fermi equation and we derive almost sharp spectral asymptotics.

Furthermore, in Section 26.5 we analyze in the case $M \ge 2$ the *boundary strip* $\{W^{\mathsf{TF}} + \nu \lesssim B\}$ containing the boundary of $\mathsf{supp}(\rho_B^{\mathsf{TF}})$; this is the most difficult case to analyze and our remainder estimates are not sharp unless $N \ge Z - CZ^{\frac{2}{3}}$.

Finally, in Section 26.6 we derive asymptotics of the ground state energy. Their precision (or lack of it) follows from the precision of the corresponding semiclassical results; so our results in the case $M = 1$ are sharp, but our results in the case $M \ge 2$ (especially if $N \le Z - CZ^{\frac{2}{3}}$) are not.

In the second half of this Chapter we consider related problems. In Section 26.7 (cf. Section 25.5) we consider negatively charged systems ($N \ge Z$) and estimate both ionization energy I_N and excessive negative charge $(N - Z)_+$ [4)].

In Section 26.8 (cf. Section 25.6) we consider positively charged systems ($N \le Z$) and estimate the remainder $|\mathsf{I}_N + \nu|$ in the formula $\mathsf{I}_N \approx -\nu$; for $M \ge 2$ we also consider a free nuclei model and estimate from below the distance between nuclei and an excessive positive charge $(Z - N)_+$ when atoms can be bound into molecule[4)].

[4)] In the (magnetic) Thomas-Fermi theory both answers are 0.

Appendices contain some auxiliary material, most notably, electrostatic inequalities in Appendix 26.A.1 and also Zhislin's theorem (that system can bind at least Z electrons) in Appendix 26.A.4–all in the case of magnetic field.

26.2 Magnetic Thomas-Fermi Theory

26.2.1 Framework and Existence

The Thomas-Fermi theory is well developed in the magnetic case as well albeit in the lesser degree than in the non-magnetic one. The most important source now is Section IV of E. H. Lieb, J. P. Solovej and J. Yngvason [3].

Again as in the previous Chapter 25 to get the best lower estimate for the ground state energy (neglecting semiclassical errors) one needs to maximize functional $\Phi_{B,*}(W+\nu)$ defined by (25.3.1) albeit with the pressure $P_B(w)$ given for $d=2,3$ by (26.1.19). Formulae (25.3.2) and (25.3.3) also remain valid.

Further, to get the best upper estimate (neglecting semiclassical errors) one needs to minimize functional $\Phi^*_B(\rho',\nu)$ defined by (25.3.4) where (25.3.4) remains valid with P replaced by P_B and respectively $\tau(\rho')$ replaced by $\tau_B(\rho')$ which is Legendre transformation of P_B (see (26.1.18)).

Since P_B is given by much more complicated expression (26.1.19) rather than $(25.3.6)_1$, and respectively

$$P'_B(w)=\frac{d}{2}\varkappa_1 B\Bigl(\frac{1}{2}w_+^{\frac{d}{2}-1}+\sum_{j\geq 1}(w-2jB)_+^{\frac{d}{2}-1}\Bigr) \tag{26.2.1}$$

(cf. $(25.3.6)_2$), there is no explicit expression for τ_B similar to (25.3.7).

Remark 26.2.1. (i) $B(x)=|\nabla\times A(x)|$.

(ii) From now on we will assume that $d=3$.

(iii) P_B is a strictly convex function and therefore τ_B is also a strictly convex function[5].

[5] As $d=2$, P_B is a convex and piecewise linear function and therefore τ_B is also a convex function.

(iv) $P_B(w)\to P_0(w)$, $P'_B(w)\to P'_0(w)$ and $\tau_B(\rho)\to\tau_0(\rho)$ as $B\to 0$ where (without subscript "0") the limit functions have been defined by $(25.3.6)_{1,2}$ and (25.3.7) respectively.

Remark 26.2.2. (i) Alternatively we minimize $\mathcal{E}_B(\rho)=\Phi^*_B(\rho,0)$ under assumptions

$$\rho\ge 0,\qquad \int \rho\,dx\le N. \tag*{$(26.2.2)_{1,2}$}$$

(ii) So far in comparison with the previous Chapter 25 we changed only definition of $P_B(w)$ and $\tau_B(\rho)$ respectively. Note that $P_B(w)$ belongs to $\mathscr{C}^{\frac{d}{2}+1}$ (as $d=2,3$) as function of w; this statement will be quantified later.

(iii) While not affecting existence (with equality in $(26.2.2)_1$ iff $N\le Z$) and uniqueness of solution, it affects other properties, especially as $B\ge Z^{\frac{4}{3}}$.

Proposition 26.2.3. *In our assumptions for any fixed $\nu\le 0$ Statements (i)–(viii) of Proposition 25.3.1 hold.*

Proof. The proof is the same as of Proposition 25.3.1. The proof that threshold $\nu=0$ matches to $N=Z$ are theorems 4.9 and 4.10 of Section IV of E. H. Lieb, J. P. Solovej and J. Yngvason [3]. □

Note that (25.3.8)–(25.3.9) and (25.3.10) become

$$\rho=\frac{1}{4\pi}\Delta(W-V)=P'_B(W+\nu), \tag{26.2.3}$$

$$W=o(1)\qquad\text{as }\ |x|\to\infty \tag{26.2.4}$$

and

$$\mathcal{N}(\nu)=\int P'_B(W+\nu)\,dx \tag{26.2.5}$$

respectively.

Similarly, Proposition 25.3.2 remains true:

Proposition 26.2.4. *For arbitrary W the following estimates hold with absolute constants $\epsilon_0>0$ and C_0:*

$$\epsilon_0\mathsf{D}(\rho-\rho^{\mathsf{TF}},\rho-\rho^{\mathsf{TF}})\le\Phi_{B,*}(W^{\mathsf{TF}}+\nu)-\Phi_{B,*}(W+\nu)\le C_0\mathsf{D}(\rho-\rho',\rho-\rho') \tag{26.2.6}$$

and

$$\epsilon_0 \mathsf{D}(\rho' - \rho^{\mathsf{TF}}, \rho' - \rho^{\mathsf{TF}}) \le \Phi^*_B(\rho, \nu) - \Phi^*_B(\rho^{\mathsf{TF}}, \nu) \le C_0 \mathsf{D}(\rho - \rho', \rho - \rho') \tag{26.2.7}$$

with $\rho = \frac{1}{4\pi}\Delta(W - V)$, $\rho' = P'_B(W + \nu)$.

Proof. This proof is rather obvious as well. □

26.2.2 Properties

Proposition 26.2.5. *The solution of the magnetic Thomas-Fermi problem has the following scaling properties*

$$W^{\mathsf{TF}}(x;\, \underline{Z};\, \underline{y};\, B;\, N;\, q) = q^{\frac{2}{3}} N^{\frac{4}{3}} W^{\mathsf{TF}}(q^{\frac{2}{3}} N^{\frac{1}{3}} x;\, N^{-1}\underline{Z};\, q^{\frac{2}{3}} N^{\frac{1}{3}} \underline{\mathsf{y}};\, q^{-\frac{2}{3}} N^{-\frac{4}{3}} B;\, 1; 1), \tag{26.2.8}$$

$$\rho^{\mathsf{TF}}(x;\, \underline{Z};\, \underline{y};\, B;\, N;\, q) = q^2 N^2 \rho^{\mathsf{TF}}(q^{\frac{2}{3}} N^{\frac{1}{3}} x;\, N^{-1}\underline{Z};\, q^{\frac{2}{3}} N^{\frac{1}{3}} \underline{\mathsf{y}};\, q^{-\frac{2}{3}} N^{-\frac{4}{3}} B;\, 1; 1), \tag{26.2.9}$$

$$\mathcal{E}^{\mathsf{TF}}(\underline{Z};\, \underline{y};\, B;\, N;\, q) = q^{\frac{2}{3}} N^{\frac{7}{3}} \mathcal{E}^{\mathsf{TF}}(N^{-1}\underline{Z};\, q^{\frac{2}{3}} N^{\frac{1}{3}} \underline{\mathsf{y}};\, q^{-\frac{2}{3}} N^{-\frac{4}{3}} B;\, 1;\, 1), \tag{26.2.10}$$

$$\nu^{\mathsf{TF}}(\underline{Z};\, \underline{y};\, B;\, N;\, q) = q^{\frac{2}{3}} N^{\frac{4}{3}} \nu^{\mathsf{TF}}(N^{-1}\underline{Z};\, q^{\frac{2}{3}} N^{\frac{1}{3}} \underline{\mathsf{y}};\, q^{-\frac{2}{3}} N^{-\frac{4}{3}} B;\, 1;\, 1) \tag{26.2.11}$$

where $\nu^{\mathsf{TF}} = \nu$ *is the chemical potential; recall that* $\underline{Z} = (Z_1, \dots, Z_M)$ *and* $\underline{\mathsf{y}} = (\mathsf{y}_1, \dots, \mathsf{y}_M)$ *are arrays and parameter* q *also enters into Thomas-Fermi theory.*

In particular, ν^{TF} *and* B *scale the same way.*

Proof. Proof is trivial by scaling. □

Now one can guess that there are two cases $B \ll Z^{\frac{4}{3}}$ and $B \gg Z^{\frac{4}{3}}$ (recall that $N \asymp Z$) in which magnetic Thomas-Fermi theory looks very different (and also an intermediate case $B \sim Z^{\frac{4}{3}}$). To explain this difference let us consider one atom case:

First of all recall that if $B = 0$ and $N = Z$ theory (as $M = 1$) has just one parameter and we can get rid of it by rescaling; $W^{\mathsf{TF}} \asymp Z\ell^{-1}$ as $\ell \lesssim Z^{-\frac{1}{3}}$ <u>and</u> $W^{\mathsf{TF}} \asymp \ell^{-4}$ as $\ell \gtrsim Z^{-\frac{1}{3}}$. Then

$$\mathsf{W}^{\mathsf{TF}\,\frac{3}{2}}\ell^3 \asymp Z^{\frac{3}{2}}\ell^{\frac{3}{2}}, \quad \mathsf{W}^{\mathsf{TF}\,\frac{5}{2}}\ell^3 \asymp Z^{\frac{5}{2}}\ell^{\frac{1}{2}}$$

and

$$\mathsf{W}^{\mathsf{TF}\,\frac{3}{2}}\ell^3 \asymp \ell^{-3}, \quad \mathsf{W}^{\mathsf{TF}\,\frac{5}{2}}\ell^3 \asymp \ell^{-7}$$

respectively where the first factors are spacial densities of the charge and (negative) Thomas-Fermi energy respectively and therefore zone $\ell \asymp Z^{-\frac{1}{3}}$ provides the main contributions into both.

Therefore, if in this *main zone* $B \ll W^{\mathsf{TF}} \asymp Z^{\frac{4}{3}}$ we guess that the magnetic theory is similar to non-magnetic one, and actually it is true.

However, let us study an atomic case rigorously. Let $M = 1$, $\mathsf{y}_m = 0$ and $N \le Z$. Then

(26.2.12) W_B^{TF} is a spherically symmetric, and it is monotone non-increasing function of $|x|$; $W_B^{\mathsf{TF}} \to +0$ as $|x| \to \infty$;

$$W_B^{\mathsf{TF}}(x) \le -\nu \implies W_B^{\mathsf{TF}} = |x|^{-1}(Z - N). \tag{26.2.13}$$

Indeed, (26.2.12) is obvious and (26.2.13) follows from it and Newton screening theorem.

Two propositions below treat cases $B \lesssim Z^{\frac{4}{3}}$ and $B \gtrsim Z^{\frac{4}{3}}$ respectively; in the former case there is another fork: $B \lesssim (Z-N)_+^{\frac{4}{3}}$ and $B \gtrsim (Z-N)_+^{\frac{4}{3}}$.

Proposition 26.2.6. *Let $M = 1$, $\mathsf{y}_m = 0$, $N \asymp Z_m$ and $B \le Z^{\frac{4}{3}}$.*

(i) Then

$$W_B^{\mathsf{TF}} \le \min(Z|x|^{-1}, C|x|^{-4}) \tag{26.2.14}$$

and

$$\rho_B^{\mathsf{TF}} \le C\min(Z^{\frac{3}{2}}|x|^{-\frac{3}{2}} + BZ^{\frac{1}{2}}|x|^{-\frac{1}{2}}, |x|^{-6} + B|x|^{-2}). \tag{26.2.15}$$

(ii) There exists

$$\bar{r}_m \asymp \min\bigl(B^{-\frac{1}{4}}, (Z-N)_+^{-\frac{1}{3}}\bigr) \tag{26.2.16}$$

such that $W_B^{\mathsf{TF}} \gtrless -\nu$ as $|x| \lessgtr \bar{r}_m$ and then $\rho_B^{\mathsf{TF}} = 0$ iff $x \ge \bar{r}_m$.

(iii) (26.2.14) *and* (26.2.15) *become equivalencies ($\asymp$) as $|x| \le (1-\epsilon)\bar{r}_m$.*

(iv) $B\le (Z-N)_+^{\frac{4}{3}}$ *implies* $\bar{r}_m\asymp (Z-N)_+^{-\frac{1}{3}}$, $\nu\asymp (Z-N)_+^{\frac{4}{3}}$ *and*

$$\begin{aligned} W^{\mathsf{TF}}+\nu &\asymp (Z-N)_+^{\frac{5}{3}}(\bar{r}_m-|x|),\\ -\partial_{|x|}W^{\mathsf{TF}} &\asymp (Z-N)_+^{\frac{5}{3}} \qquad\qquad \textit{if}\ \ (1-\epsilon)\bar{r}_m\le |x|\le \bar{r}_m. \end{aligned}\tag{26.2.17}$$

(v) $B\ge (Z-N)_+^{\frac{4}{3}}$ *implies* $\bar{r}_m\asymp B^{-\frac{1}{4}}$, $\nu\asymp (Z-N)_+B^{\frac{1}{4}}\lesssim B$ *and*

$$\begin{aligned} W^{\mathsf{TF}}+\nu &\asymp B^2(\bar{r}_m-|x|)^4+B^{\frac{1}{2}}(Z-N)_+(\bar{r}_m-|x|)\\ -\partial_{|x|}W^{\mathsf{TF}} &\asymp B^2(\bar{r}_m-|x|)^3+B^{\frac{1}{2}}(Z-N)_+\\ &\qquad\qquad \textit{as}\quad (1-\epsilon)\bar{r}_m\le |x|\le \bar{r}_m. \end{aligned}\tag{26.2.18}$$

Proposition 26.2.7. *Let* $M=1$, $\mathsf{y}_m=0$, $N\asymp Z_m$ *and* $B\ge Z^{\frac{4}{3}}$.

(i) Then

$$W_B^{\mathsf{TF}}\le Z|x|^{-1}\tag{26.2.19}$$

and

$$\rho_B^{\mathsf{TF}}\le CZ^{\frac{3}{2}}|x|^{-\frac{3}{2}}+CBZ^{\frac{1}{2}}|x|^{-\frac{1}{2}}.\tag{26.2.20}$$

(ii) There exist $\bar{r}_m$ *and* $\bar{r}'_m$,

$$\bar{r}_m\asymp B^{-\frac{2}{5}}Z^{\frac{1}{5}},\qquad \bar{r}'_m\asymp B^{-1}Z_m,\tag{26.2.21}$$

such that $W_B^{\mathsf{TF}}\gtrless B$ *as* $|x|\lessgtr \bar{r}_m$, $W_B^{\mathsf{TF}}\gtrless -\nu$ *as* $|x|\lessgtr \bar{r}'_m$ *and then* $\rho_B^{\mathsf{TF}}=0$ *iff* $x\ge \bar{r}_m$.

(iii) (26.2.19)–(26.2.20) *become equivalencies* ($\asymp$) *as* $|x|\le (1-\epsilon)\bar{r}_m$.

(iv) $\nu\asymp (Z-N)_+B^{\frac{2}{5}}Z^{-\frac{1}{5}}\lesssim B$ *and*

$$W^{\mathsf{TF}}+\nu\asymp B^2(\bar{r}_m-|x|)^4+\bar{r}_m^{-2}(Z-N)_+(\bar{r}_m-|x|)\tag{26.2.22}$$

and

$$-\partial_{|x|}W^{\mathsf{TF}}\asymp B^2(\bar{r}_m-|x|)^3+\bar{r}_m^{-2}(Z-N)_+\tag{26.2.23}$$

as $(1-\epsilon)\bar{r}_m\le |x|\le \bar{r}_m$.

Proofs of Propositions 26.2.6 and 26.2.7. Proofs easily follow from equation and "boundary conditions" satisfied by $w(r)$ where $r=|x|$:

$$w''+2r^{-1}w=P'_B(w+\nu), \tag{26.2.24}$$

$$w=r^{-1}Z_m+O(1)\qquad \text{as}\quad r\to 0, \tag{26.2.25}$$

$$w(\bar{r}_m)=-\nu,\qquad w'(\bar{r}_m)=\nu\bar{r}_m^{-1} \tag{26.2.26}$$

where $\nu=-(Z_m-N)_+\bar{r}_m^{-1}$. □

Corollary 26.2.8. *Let $M=1$, $\mathsf{y}_m=0$ and $N\asymp Z_m$. Then*

(i) $W_B^{\mathsf{TF}}\lesssim B$ if $|x|\ge\bar{r}'_m$ where $\bar{r}'_m\asymp B^{-1}Z_m$ as $B\ge Z_m^{\frac{4}{3}}$ and $\bar{r}'_m\asymp B^{-\frac{1}{4}}$ as $B\le cZ_m^{\frac{4}{3}}$.

(ii) As $B\lesssim Z_m^{\frac{4}{3}}$ the main contribution to both the charge and the Thomas-Fermi energy is delivered by zone $\{x\colon |x|\asymp r_m^*\}$ with $r_m^*=Z_m^{-\frac{1}{3}}$; in particular, then $\mathcal{E}_B^{\mathsf{TF}}\asymp\mathcal{E}^{\mathsf{TF}}\asymp Z_m^{\frac{7}{3}}$; further, in this case $W_B^{\mathsf{TF}}\asymp W^{\mathsf{TF}}$ in the zone $\{x\colon |x|\lesssim\epsilon\bar{r}_m\}$.

(iii) Further, $\mathcal{E}_B^{\mathsf{TF}}\sim\mathcal{E}^{\mathsf{TF}}$ as $B\ll Z_m^{\frac{4}{3}}$; furthermore, in this case $W_B^{\mathsf{TF}}\sim W^{\mathsf{TF}}$ in the zone $\{x\colon |x|\ll\bar{r}_m\}$.

(iv) On the other hand, as $B\ge Z^{\frac{4}{3}}$, the main contributions to the total charge and energy are delivered by $\{x\colon |x|\asymp\bar{r}_m\}$ and in particular $\rho_m\asymp BZ_m^{\frac{1}{2}}\bar{r}_m^{\frac{5}{2}}$ and

$$\mathcal{E}_B^{\mathsf{TF}}\asymp BZ_m^{\frac{3}{2}}\bar{r}_m^{\frac{3}{2}}\asymp B^{\frac{2}{5}}Z_m^{\frac{9}{5}}. \tag{26.2.27}$$

Recall that $\bar{r}_m\asymp B^{-\frac{1}{4}}$ as $B\le Z_m^{\frac{4}{3}}$ and $\bar{r}_m\asymp B^{-\frac{2}{5}}Z_M^{\frac{1}{5}}$ as $B\ge Z_M^{\frac{4}{3}}$. Note that Proposition 25.3.5 (comparing W^{TF} for molecule with the sum of those for single atoms) still holds. Therefore we conclude that

Corollary 26.2.9. *(i) Assume that*

$$Z_m\asymp Z \tag{26.2.28}$$

for all $m=1,\dots,M$. Then all statements of corollary 26.2.8 remain true for $M\ge 2$ with $|x|$ and Z_m replaced by $\ell(x)$ and Z and $\bar{r}_m$, $\bar{r}'_m$, r_m^* by $\bar{r}$, $\bar{r}'$, r^* respectively.

(ii) In the general case global statements remain true, pointwise statements remain true without modification only as $\ell(x) = \ell_m(x) := |x - \mathsf{y}_m|$ *with* $Z_m \asymp Z$.

Remark 26.2.10. (i) Also holds Proposition 25.3.13 as it uses only super-additivity of $\tau(\rho)$ and $\tau_B(\rho)$ is also super-additive (this follows from convexity of $\tau_B(\rho)$ and equality $\tau_B(0) = 0$).

(ii) However there is a significant difference: if there is no magnetic field atoms really repulse one another on any distances and we can attribute it to either excessive positive charge as $N < Z$ or their infinite spatial size as $N = Z$. However with magnetic field atoms have a finite size even as $N = Z$ and they do not repulse one another on the large distances. In particular, Proposition 26.2.11 below holds.

Proposition 26.2.11. *Let* $N = Z$ *and*

$$|\mathsf{y}_m - \mathsf{y}_{m'}| \ge \bar{r}_m + \bar{r}_{m'} \qquad \forall m:\ 1 \le m < m' \le M. \tag{26.2.29}$$

Then

$$\mathcal{E}_B^{\mathsf{TF}}(\underline{Z}, \underline{\mathsf{y}}, B, Z) = \sum_{1\le m\le M} \mathcal{E}_B^{\mathsf{TF}}(Z_m, \mathsf{y}_m, B, Z_m) \tag{26.2.30}$$

and

$$\rho_B^{\mathsf{TF}}(x, \underline{Z}, \underline{\mathsf{y}}, B, Z) = \sum_{1\le m\le M} \rho_B^{\mathsf{TF}}(x, Z_m, \mathsf{y}_m, B, Z_m). \tag{26.2.31}$$

Proposition 26.2.12. *(i)* ν *is monotone increasing function of* N.

(ii) $W_B(x)$ *is monotone non-increasing function of* N.

(iii) $W_B(x) + \nu$ *is monotone non-decreasing function of* N *; in particular* ρ_B *can only increase as* N *increases.*

(iv) ν *is monotone non-increasing function of* Z_m.

(v) $W_B(x)$ *is monotone non-decreasing function of* Z_m.

Proof. (i) Statement (i) follows from the strict convexity of $\mathcal{E}(\rho)$: consider two solutions with corresponding subscripts. Then $\mathcal{E}(\rho) - \mathcal{E}(\rho_j) > \nu_j(N - N_j)$ for any non-negative $\rho \ne \rho_j$ and $N = \int \rho\, dx$.

In particular, $\mathcal{E}(\rho_1) - \mathcal{E}(\rho_2) > \nu_2(N_1 - N_2)$ and $\mathcal{E}(\rho_2) - \mathcal{E}(\rho_1) > \nu_1(N_2 - N_1)$ and then $(\nu_1 - \nu_2)(N_1 - N_2) > 0$.

(ii) Indeed, consider $N_1 < N_2$ and in the definition of W_2 slightly decrease $Z_1, \dots, Z_M$ thus replacing them by $Z'_1, \dots, Z'_M$. Then $W_1 > W_2$ for large $|x|$, $W_1 - W_2 \to +\infty$ as $x \to \mathsf{y}_m$ and therefore if Statement (ii) fails, then $W_1 - W_2$ reaches non-positive minimum at some regular point $\bar{x}$; at this point $W_1 \le W_2$ and

$$0 \le \frac{1}{4\pi}\Delta(W_1 - W_2) = P'(W_1 + \nu_1) - P'(W_2 + \nu_2).$$

This is possible only if at this point $W_2 + \nu_2 \le 0$ and $W_1 + \nu_1 < 0$. Then in the small vicinity $\Delta(W_1 - W_2) \le 0$ and $\bar{x}$ cannot be a point of minimum unless $W_1 - W_2 = \mathsf{const}$ there. Then any point of this vicinity is also a point of minimum and then due to standard analytic arguments $W_1 - W_2 = \mathsf{const}$ everywhere which is impossible.

So, $W_1(x; Z_1, \dots, Z_M) > W_2(x; Z'_1, \dots, Z'_M)$. Taking limit as $Z'_m \to Z_m$ we arrive to $W_1(x; Z_1, \dots, Z_M) \ge W_2(x; Z_1, \dots, Z_M)$.

(iii) Proof of Statement (iii) is similar but roles of W_1 and W_2 are played by $W_2 + \nu_2$ and $W_1 + \nu_1$ respectively.

(iv) Let $Z_{m,2} > Z_{m,1}$ for all m. Assume that $\nu_2 > \nu_1$. Then similar arguments prove that $W_2 + \nu_2 \ge W_1 + \nu_1$ and thus $\rho_2 \ge \rho_1$ everywhere which is impossible unless there are just identical equalities as $W_2 + \nu_2 > 0$, which is impossible.

(v) Finally, after Statement (iv) was established, the same arguments prove Statement (v). □

As far as we know Theorem 1 of R. Benguria [1] (see Theorem 25.3.8) has not been proven in the case of magnetic field; however one can see easily that arguments of of R. Benguria's proof remain valid and we arrive to

Theorem 26.2.13. *All Statements (i)–(iii) of Theorem 25.3.8 hold in the case of the constant magnetic field.*

Problem 26.2.14. (i) Investigate how $\mathsf{supp}(\rho_B^{\mathsf{TF}})$ depends on B and on Z in the atomic case $M = 1$.

(ii) More generally, investigate how $\mathsf{supp}(\rho_B^{\mathsf{TF}})$ depends on B and on Z in the case $M \ge 2$.

26.2.3 Positive Ions

In view of Remark 26.2.10 we need to consider repulsion of positive ions in more details. Our purpose is to prove

Theorem 26.2.15. *Let condition* (26.2.28) *be fulfilled. Then the energy excess is estimated from below*

$$\mathcal{Q} := \widehat{\mathcal{E}}_B^{\mathsf{TF}} - \sum_{1\le m\le M} \mathcal{E}_{B,m}^{\mathsf{TF}} \ge \epsilon (Z-N)_+^2 a^{-1}. \tag{26.2.32}$$

Note first that

$$\begin{gathered}\mathsf{D}\bigl(\rho_{B(\nu)}^{\mathsf{TF}} - \rho_{B,0}^{\mathsf{TF}},\, \rho_{B(\nu)}^{\mathsf{TF}} - \rho_{B(0)}^{\mathsf{TF}}\bigr) + \\ \int \bigl(P_B'(W_{B(\nu)}^{\mathsf{TF}}+\nu) - P_B'(W_{B(0)}^{\mathsf{TF}})\bigr)\bigl(W_{B(\nu)}^{\mathsf{TF}} + \nu - W_{B(0)}^{\mathsf{TF}})\bigr)\,dx = \\ \nu \int \bigl(P_B'(W_{B(\nu)}^{\mathsf{TF}}+\nu) - P_B'(W_{B(0)}^{\mathsf{TF}}+0)\bigr)\,dx\end{gathered} \tag{26.2.33}$$

with the right-hand expression equal $\nu(N-Z) \asymp (Z-N)^2\bar{r}^{-1}$ and due to monotonicity $P_B'(w)$ we conclude that

Proposition 26.2.16. *Let condition* (26.2.28) *be fulfilled. Then*

$$\mathsf{D}\bigl(\rho_{B(\nu)}^{\mathsf{TF}} - \rho_{B(0)}^{\mathsf{TF}},\, \rho_{B,\nu}^{\mathsf{TF}} - \rho_{B(0)}^{\mathsf{TF}}\bigr) \le C(Z-N)^2\bar{r}^{-1}. \tag{26.2.34}$$

Proof of Theorem 26.2.15. Step 1. Note first that due to non-negativity of the expression

$$\widehat{\mathcal{E}}_B^{\mathsf{TF}}(\underline{Z},\underline{y},N) - \min_{N_1+N'=N}\bigl(\mathcal{E}_B^{\mathsf{TF}}(Z_1,N_1) - \widehat{\mathcal{E}}_B^{\mathsf{TF}}(\underline{Z}',\underline{y}',N')\bigr) \tag{26.2.35}$$

(see proof of Proposition 25.3.13 which persists even if there is constant magnetic field, see Remark 26.2.10) it is sufficient to prove theorem only for $M=2$. From now on we assume that $M=2$.

Step 2. According to Proposition 25.3.13

$$\mathsf{D}(\rho_B^{\mathsf{TF}} - \rho_{B,1}^{\mathsf{TF}} - \rho_{B,2}^{\mathsf{TF}}) \le C\mathcal{Q}. \tag{26.2.36}$$

Therefore due to superadditivity τ_B

(26.2.37) $$\mathcal{Q} \geq -\int V_1\rho^{\mathsf{TF}}_{B,2}\,dx - \int V_2\rho^{\mathsf{TF}}_{B,1}\,dx + \mathsf{D}(\rho^{\mathsf{TF}}_{B,2}, \rho^{\mathsf{TF}}_{B,1}) + Z_1Z_2a^{-1} - C\mathcal{Q}$$

and it is sufficient to prove the same estimate from below for the right-hand expression without the last term. However this is easy if $a \geq \bar{r}_1 + \bar{r}_2$ since $V_m = |x - \mathsf{y}_m|^{-1}Z_m$ and $\rho^{\mathsf{TF}}_{B,m} = \rho^{\mathsf{TF}}_{B,m}(|x - \mathsf{y}_m|)$ are spherically symmetric functions[6].

Therefore for $a \geq \bar{r}_1 + \bar{r}_2$ inequality (26.2.32) has been proven and in what follows we can assume that $a \leq \bar{r}_1 + \bar{r}_2$. Further, applying Theorem 26.2.13 we conclude then that

(26.2.38) Inequality (26.2.32) holds for $a \geq \epsilon\bar{r}$.

Step 3. Recall that the bulk of electrons are in the zone $\{\ell(x) \asymp r^*\}$[7]. Based on this one can prove easily that as $a \leq \epsilon\bar{r}$ the right-hand hand expression of (26.2.37) is greater than $(1-\epsilon_1)a^{-1}Z_1Z_2$ and therefore

(26.2.39) As $B \geq Z^{\frac{4}{3}}$ and $a \leq \epsilon r^*$ we have $\mathcal{Q} \geq (1-\epsilon_1)a^{-1}Z_1Z_2$

and combining with (26.2.38) we conclude that (26.2.32) holds for $B \gtrsim Z^{\frac{4}{3}}$ and for $B \lesssim Z^{\frac{4}{3}}$ we need to consider the case $\epsilon_0 r^* \leq a \leq \epsilon\bar{r}$ with arbitrarily small constant ϵ.

Replacing then P_B by P_0 and noting that an error will not exceed $C_0\bar{r}B^2 \leq C_1\epsilon a^{-7}$ while $\mathcal{Q} \geq \epsilon_0 a^{-7}$ for $B = 0$ we conclude that (26.2.32) holds as $\epsilon_0 r^* \leq a \leq c\bar{r}$ and $(Z - N) \leq C_2 a^{-3}$.

Finally, as $(Z - N) \geq C_2a^{-3}$ we see that $\bar{r} \leq C_0(Z-N)^{-\frac{1}{3}} \leq \epsilon a$ and (26.2.32) holds again. □

Even if we do not need it for our purposes we want to consider the repulsion of too close neutral atoms:

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[6] However this is not true in general as $a < \bar{r}_1 + \bar{r}_2$. Really, consider $N_m = Z_m$ and uniformly charged spheres. Then the right-hand expression of (26.2.37) is 0 as $a \geq \bar{r}_1 + \bar{r}_2$ and is negative and decays as a decays from $\bar{r}_1 + \bar{r}_2$ to $\max(\bar{r}_1, \bar{r}_2)$ and it increases again as a decays from $\max(\bar{r}_1, \bar{r}_2)$ to 0.

[7] I.e. zone $\{c(\epsilon)^{-1}r^* \leq \ell(x) \leq c(\epsilon)r^*\}$ contains at least $(1-\epsilon)N$ electrons.

Theorem 26.2.17. *Let condition* (26.2.28) *be fulfilled and* $N = Z$. *Then as* $a \geq \epsilon \bar{r}$ *the energy excess is estimated from below*

$$\mathcal{Q} \geq \epsilon G^2 \bar{r} \sum_{1\leq m<m'\leq M} (\bar{r}_m + \bar{r}_n - |\mathsf{y}_m - \mathsf{y}_{m'}|)_+^{12} \bar{r}^{-12} \tag{26.2.40}$$

where

$$G := \begin{cases} B & \text{if } B \leq Z^{\frac{4}{3}}, \\ Z^{\frac{4}{5}} B^{\frac{2}{5}} & \text{if } B \geq Z^{\frac{4}{3}}. \end{cases} \tag{26.2.41}$$

and correspondingly $G^2 \bar{r} = \begin{cases} B^{\frac{7}{4}} & \text{if } B \leq Z^{\frac{4}{3}}, \\ Z^{\frac{9}{5}} B^{\frac{2}{5}} & \text{if } B \geq Z^{\frac{4}{3}}. \end{cases}$

Proof. Again we need to consider case $M = 2$. Since

$$\frac{1}{4\pi} \Delta W_B = \rho_B - \sum_{m=1,2} Z_m \delta(x - \mathsf{y}_m) \tag{26.2.42}$$

and $W_{B,1}$, $W_{B,2}$ satisfy similar equations, (26.2.36) implies that

$$\|\nabla (W_B - W_{B,1} - W_{B,2})\| \leq c \mathcal{Q}^{\frac{1}{2}}. \tag{26.2.43}$$

This inequality and the fact that $W_B = 0$ as $\ell(x) \geq c\bar{r}$, and $W_{B,m} = 0$ as $|x - \mathsf{y}_m| \geq \bar{r}_m$ imply that

$$\|(W_B - W_{B,1} - W_{B,2})\| \leq c\bar{r} \mathcal{Q}^{\frac{1}{2}}. \tag{26.2.44}$$

Note that $\int (-\rho_B + \rho_{B,1} + \rho_{B,2})\, dx = 0$ implies that

$$|\int \bigl((W_{B,1} + W_{B,2})^{\frac{1}{2}} - W_{B,1}^{\frac{1}{2}} - W_{B,1}^{\frac{1}{2}}\bigr)\, dx \leq \int |W_B^{\frac{1}{2}} - (W_{B,1} + W_{B,2})^{\frac{1}{2}}|\, dx. \tag{26.2.45}$$

One can calculate easily that the left-hand expression has a magnitude $(G\eta^4)^{\frac{1}{2}} \cdot \eta \bar{r} \cdot (\eta^{\frac{1}{2}} \bar{r})^2 \asymp G^{\frac{1}{2}} \bar{r}^3 \eta^4$ where the first factor is a magnitude of an integrand as $W_{B,1} \asymp W_{B,2} \asymp G\eta^4$, $\eta\bar{r}$ is a depth, and $\eta^{\frac{1}{2}}\bar{r}$ the width of this zone.

On the other hand, consider the right hand expression. It consists of contributions of several zones:

(a) Zone $\mathcal{Y}_t$ where $W_{B,1} + W_{B,2} \le Gt^4$, $W_B \le 2Gt^4$. This contribution does not exceed $CG^{\frac{1}{2}} t^2 \operatorname{mes}(\mathcal{Y}_t) \asymp CG^{\frac{1}{2}} \bar{r}^3 t^3$ [8].

(b) Zone $\mathcal{Z}_t$ where $W_{B,1} + W_{B,2} \le Gt^4$, $W_B \ge 2Gt^4$. Its contribution does not exceed

$$C\int_{\mathcal{Z}_t} W_B^{\frac{1}{2}}\, dx \le C\|W_B\|_{\mathcal{Z}}^{\frac{1}{2}} (\operatorname{mes}(\mathcal{Z}_t))^{\frac{3}{4}} \le C\bar{r}^{\frac{11}{4}} \mathcal{Q}^{\frac{1}{4}} t^{\frac{3}{4}}$$

since due to (26.2.44) $\|W_B\|_{\mathcal{Z}_t} \le c\bar{r}\mathcal{Q}^{\frac{1}{2}}$.

(c) Zone where $W_{B,1} + W_{B,2} \asymp G\tau^4$. This contribution does not exceed

$$CG^{-\frac{1}{2}}\tau^{-2} \int |W_B - W_{B,1} - W_{B,2}|\, dx \le \\ CG^{-\frac{1}{2}}\tau^{-2} \times \|W_B - W_{B,1} - W_{B,2}\| \times (\operatorname{mes}(\mathcal{X}_\tau))^{\frac{1}{2}} \asymp CG^{-\frac{1}{2}} \mathcal{Q}^{\frac{1}{2}} \bar{r}^{\frac{5}{2}} \tau^{-\frac{3}{2}}. \tag{26.2.46}$$

Integrating by $\tau^{-1}\, d\tau$ from t we get (26.2.46) calculated as $\tau = t$ (and capped by the same expression as $\tau = \eta$.

So, the right-hand expression of (26.2.45) does not exceed

$$CG^{\frac{1}{2}} \bar{r}^3 t^3 + C\mathcal{Q}^{\frac{1}{4}} \bar{r}^{\frac{11}{4}} t^{\frac{3}{4}} + CG^{-\frac{1}{2}} \mathcal{Q}^{\frac{1}{2}} \bar{r}^{\frac{5}{2}} t^{-\frac{3}{2}};$$

optimizing with respect to $t = G^{-\frac{2}{9}} \mathcal{Q}^{\frac{1}{9}} \bar{r}^{-\frac{1}{9}}$ we get all three terms equal to $CG^{-\frac{1}{6}} Q^{\frac{1}{3}} \bar{r}^{\frac{8}{3}}$ comparing with $CG^{\frac{1}{2}} \bar{r}^3 \eta^4$ we arrive to (26.2.40). □

26.3 Applying Semiclassical Methods: $M = 1$

26.3.1 Heuristics

Let us consider first a mock proof of our main results; we deal here *as if* W_B^{TF} *was very smooth* which it is not the case; however later we will show that its smoothness is sufficient to employ arguments of Chapter 18 rather than those of Chapter 13. We also will deal as if non-degeneracy conditions were satisfied leaving them also to more rigorous arguments below.

It will allow us to establish our target remainder estimates which we will be able to prove rigorously for $M = 1$ (in this section) while for $M \ge 2$ (in the next two sections) our results will be not that good.

[8] Obviously, $\operatorname{mes}(\mathcal{Y}_t \cup \mathcal{Z}_t) \asymp \bar{r}^3 t$ and similarly $\operatorname{mes}(\mathcal{X}_\tau) \asymp \bar{r}^3 \tau$.

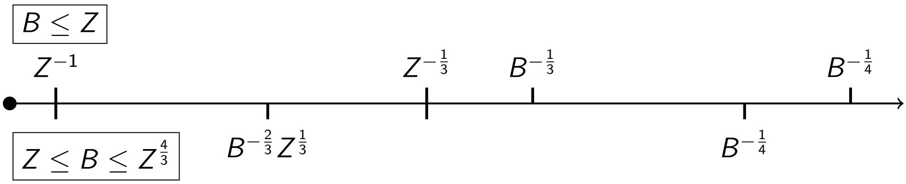

Figure 26.1: Let $B \le Z^{\frac{4}{3}}$. Then at $\{\ell \asymp Z^{-\frac{1}{3}}\}$ are contained both the bulk of charge and the bulk of energy, $\ell \asymp \min((Z-N)_+^{-\frac{1}{3}}, B^{-\frac{1}{4}}\}$ is the border of $\mathsf{supp}(\rho_B^{\mathsf{TF}})$; $\ell \asymp Z^{-1}$ is the Scott distance; here $h \asymp 1$. Further, $\ell \asymp B^{-\frac{1}{3}}$ if $B \le Z$ and $\ell \asymp B^{-\frac{2}{3}}Z^{\frac{1}{3}}$ if $Z \le B \le Z^{\frac{4}{3}}$ separates $\{\mu \lesssim 1\}$ (on the left) and $\{\mu \gtrsim 1\}$ (on the right).

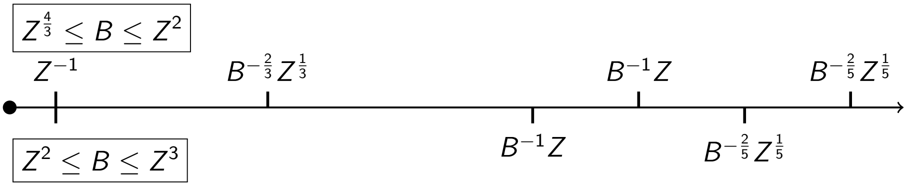

Figure 26.2: Let $Z^{\frac{4}{3}} \le B \le Z^3$. Then at $\{\ell \asymp Z^{-\frac{2}{5}}B^{\frac{1}{5}}\}$ are contained both the bulk of charge and the bulk of energy and it is also the border of $\mathsf{supp}(\rho_B^{\mathsf{TF}})$; $\ell \asymp Z^{-1}$ is the Scott distance; here $h \asymp 1$. Further, if $Z^{\frac{4}{3}} \le B \le Z^2$ $\ell \asymp B^{-\frac{2}{3}}Z^{\frac{1}{3}}$ separates $\{\mu \lesssim 1\}$ (on the left) and $\{\mu \gtrsim 1\}$ (on the right) and $\ell \asymp B^{-1}Z$ separates $\{\mu h \lesssim 1\}$ (on the left) and $\{\mu h \gtrsim 1\}$ (on the right).

Total Charge

Consider

$$\int e(x,x,\nu)\psi(x)\,dx, \tag{26.3.1}$$

first with γ-admissible $\psi(x)$, where $\gamma \le \epsilon\ell$. Recall that $\ell(x) = \min_m |x - y_m|$ is the distance to the nearest nucleus.

General Arguments. The main part of the semiclassical expression for (26.3.1) is of magnitude $h'^{-3} + \mu' h'^{-2} \asymp \zeta^3\gamma^3 + B\zeta\gamma^3$ with $h' = 1/(\zeta\gamma)$ and $\mu' = B\gamma/\zeta$.

Indeed, let us rescale $x\mapsto x/\gamma$ and $\tau\mapsto\tau/\zeta^2$ which leads to $h=1\mapsto h'$ and $B\mapsto\mu'$. In particular, for $\gamma\asymp\ell$ we get

$$\zeta^3\ell^3+B\zeta\ell^3. \tag{26.3.2}$$

Meanwhile, the remainder in the semiclassical expression for (26.3.1) does not exceed $Ch'^{-2}+C\mu'h'^{-1}\asymp\zeta^2\gamma^2+B\gamma^2$ (gaining factor h' in comparison to the main part; here we need the smoothness and if $\mu'\geq h'^{\delta-1}$ we also need the non-degeneracy); for $\gamma\asymp\ell$ we get

$$\zeta^2\ell^2+B\ell^2. \tag{26.3.3}$$

Sure, we ignored the fact that $h'\leq 1$ does not necessarily hold even if $\gamma\asymp\ell$ but we believe that the contributions to the main part and the remainder of these zones will be less than of zone where this inequality holds, provided $B\ll Z^3$.

Finally, let us sum expressions (26.3.2) and (26.3.3) with respect to ℓ-partition.

Moderate Magnetic Field. Consider the case $B\leq Z^{\frac{4}{3}}$ first. Then for $\ell\leq Z^{-\frac{1}{3}}$ we plug $\zeta=Z^{\frac{1}{2}}\ell^{-\frac{1}{2}}$ into (26.3.2) and (26.3.3) resulting in

$$Z^{\frac{3}{2}}\ell^{\frac{3}{2}}+BZ^{\frac{1}{2}}\ell^{\frac{5}{2}}\qquad\text{and}\qquad Z\ell+B\ell^2 \tag*{(26.3.4)$_{0,1}$}$$

in the main part and in the remainder respectively and the summation over zone $\{x\colon \ell(x)\leq Z^{-\frac{4}{3}}\}$ results in the same expressions with $\ell=Z^{-\frac{1}{3}}$, i. e. in $Z+BZ^{-\frac{1}{3}}\asymp Z$ and $Z^{\frac{2}{3}}+BZ^{-\frac{2}{3}}\asymp Z^{\frac{2}{3}}$ respectively.

On the other hand, for $\ell\geq Z^{-\frac{1}{3}}$ we plug $\zeta=\ell^{-2}$ into (26.3.2) and (26.3.3) resulting in

$$\ell^{-3}+B\ell\qquad\text{and}\qquad\ell^{-2}+B\ell^2; \tag*{(26.3.5)$_{0,1}$}$$

then summation over zone $\{x\colon Z^{-\frac{1}{3}}\leq\ell(x)\leq\bar{r}=B^{-\frac{1}{4}}\}$ results in $Z+B^{\frac{3}{4}}\asymp Z$ and $Z^{\frac{2}{3}}+B^{\frac{1}{2}}\asymp Z^{\frac{2}{3}}$ respectively.

Strong Magnetic Field. Consider the case $B\geq Z^{\frac{4}{3}}$ now. Then the threshold $Z^{-\frac{1}{3}}$ disappears and we sum expressions $(26.3.4)_{0,1}$ over zone $\{x\colon \ell(x)\leq\bar{r}\coloneqq Z^{\frac{1}{5}}B^{-\frac{2}{5}}\}$, resulting in $Z^{\frac{9}{5}}B^{-\frac{3}{5}}+Z\asymp Z$ and $Z^{\frac{6}{5}}B^{-\frac{2}{5}}+Z^{\frac{2}{5}}B^{\frac{1}{5}}\asymp Z^{\frac{2}{5}}B^{\frac{1}{5}}$ respectively.

Therefore, for both cases $B\lesseqgtr Z^{\frac{4}{3}}$ we arrive to

(26.3.6) The total charge is $\min(N, Z)$ (due to the choice of ν) with the remainder estimate $O\bigl(\max(Z^{\frac{2}{3}}, Z^{\frac{2}{5}}B^{\frac{1}{5}})\bigr)$ which is $O(Z^{\frac{2}{3}})$ if $B \le Z^{\frac{4}{3}}$ and $O(Z^{\frac{2}{5}}B^{\frac{1}{5}})$ if $Z^{\frac{4}{3}} \le B \le Z^3$.

Remark 26.3.1. Remainder is less than the main part if $Z^{\frac{2}{5}}B^{\frac{1}{5}} \lesssim Z$ i.e. $B \le Z^3$. It means exactly that $\zeta\ell \ge 1$ if $\ell = \bar{r}$ (in the case $B \ge Z^{\frac{4}{3}}$), or, in other words that $h \lesssim 1$. The same is true for all other semiclassical asymptotics below.

If $B \ll Z^3$ we arrive to asymptotics, ig $B \lesssim Z^3$ we have estimates and in the case of superstrong magnetic field $B \gg Z^3$ Thomas-Fermi theory is not valid for our main model.

Semiclassical D-Term

Consider now the semiclassical D-term

$$\mathsf{D}\bigl(e(x,x,\nu) - \rho_B^{\mathsf{TF}}(x),\ e(x,x,\nu) - \rho_B^{\mathsf{TF}}(x)\bigr). \tag{26.3.7}$$

General Arguments. We do not have appropriate asymptotics for $e(x,x,\nu)$ in the case of the magnetic field[9)] but we apply Fefferman–de Llave decomposition (16.4.1):

$$|x-y|_\gamma^{-1}(x,y) := |x-y|\varphi(\gamma^{-1}|x-y|) = \gamma^{-4}\int \psi_{1,\gamma}(x,z)\psi_{2,\gamma}(y,z)\,dz \tag{26.3.8}$$

where $\varphi \in \mathscr{C}^\infty([1,2])$.

Therefore contribution of $B(z,\gamma)\times B(z',\gamma)$ with $3\gamma \le |z-z'| \le 4\gamma$, $\gamma \le \epsilon\ell(z)$ to such term does not exceed $C\bigl(\zeta^2\gamma^2 + B\gamma^2)^2\gamma^{-1}$. There are $\asymp \ell^3\gamma^{-3}$ of such pairs with $\ell(x) \asymp \ell$ and their total contribution does not exceed $C\bigl(\zeta^2 + B)^2\ell^3$.

Now we need to sum over $\gamma^{-1}\,d\gamma$ which does not look good because it leads to the logarithmic divergency but there is a simple remedy: we treat this way only pairs $t\ell \le |z-z'| \le \ell$ and apply for pairs with $|z-z'| \le t\ell$ pointwise asymptotics; then we get

$$C(\zeta^2 + B)^2\ell^3\bigl(1 + (\log B\ell/\zeta)_+\bigr); \tag{26.3.9}$$

9) Unless we really assume that W is smooth and apply results sections 16.6–16.9.

to get rid of this logarithmic factor we apply more delicate arguments similar to those of Subsection 16.10.3.

Thus, ignoring this logarithmic factor we conclude that the contribution of all pairs (z, z') with $\ell(z) \asymp \ell(z') \asymp \ell$ does not exceed $C(\zeta^2 + B)^2\ell^3$ while contribution of all pairs (z, z') with $\ell(z) \asymp \ell_1 \not\asymp \ell(z') \asymp \ell_2$ does not exceed $C(\zeta_1^2 + B)(\zeta_2^2 + B)\ell_1^2\ell_2^2(\ell_1 + \ell_2)^{-1}$.

Finally let us sum these expressions over partitions of unity.

Moderate Magnetic Field. Consider the case $B \le Z^{\frac{4}{3}}$. Then summation over zone $\{\ell_1 \le Z^{-\frac{1}{3}}, \ell_2 \le Z^{-\frac{1}{3}}\}$ results in $CZ^{\frac{5}{3}}$ and the same is also true for summation over zone $\{Z^{-\frac{1}{3}} \le \ell_1 \le B^{-\frac{1}{4}}, Z^{-\frac{1}{3}} \le \ell_2 \le B^{-\frac{1}{4}}\}$.

Obviously, in such estimates, if there is a fixed number of zones, we do not need to sum over "mixed" pairs when z and z' belong to different zones.

Strong Magnetic Field. Consider the case $B \ge Z^{\frac{4}{3}}$. Then summation over zone $\{\ell_1 \le Z^{\frac{1}{5}}B^{-\frac{2}{5}}, \ell_2 \le Z^{\frac{1}{5}}B^{-\frac{2}{5}}\}$ results in $CZ^{\frac{3}{5}}B^{\frac{4}{5}}$.

Therefore, for both cases $B \lesseqgtr Z^{\frac{4}{3}}$ we arrive to

(26.3.10) Term (26.3.7) does not exceed $C\max(Z^{\frac{5}{3}}, Z^{\frac{3}{5}}B^{\frac{4}{5}})$ which is $CZ^{\frac{5}{3}}$ if $B \le Z^{\frac{4}{3}}$ and $CZ^{\frac{3}{5}}B^{\frac{4}{5}}$ if $Z^{\frac{4}{3}} \le B \le Z^3$.

Remark 26.3.2[10]. Estimating this term, and also the second D-term (in the next paragraph) we need to estimate the contribution of the singular zone $\{x\colon \ell(x) \le \bar{r} = Z^{-1}\}$ where effective semiclassical parameter is less than 1. We claim that there

$$e(x, x, 0) \le C(BZ + Z^3) \qquad \text{for} \ \ \lambda \le cZ^2. \tag{26.3.11}$$

Indeed, it is true if $\ell(x) \ge 1$. Also operator H is bounded from below by $-CZ^2$. And finally, in the ball of $B(\mathsf{y}_m, \epsilon Z^{-1})$ operator Δ is larger than $Z|x - \mathsf{y}_m|^{-1}$. We leave the easy details to the reader.

Therefore for $B \le Z^2$ the contribution of this zone into N-term is $O(CZ^3\bar{r}^3) = O(1)$, into both D-terms is $O(Z^6\bar{r}^5) = O(Z)$, and into T-term is $O(Z^5\bar{r}^3) = O(Z^2)$ exactly as in Chapter 25. On the other hand, for $Z^2 \le BleZ^3$ the contribution of this zone into N-term is $O(CBZ\bar{r}^3) = O(BZ^{-2})$, into both D-terms is $O(B^2Z^2\bar{r}^5) = O(B^2Z^{-3})$, and into T-term is $O(BZ^3\bar{r}^3) = O(B)$.

[10] Cf. Remark 25.4.7.

$|\lambda_N - \nu|$ and Another D-Term

Consider two other non-trace terms in the upper estimate.

Moderate Magnetic Field. In the case $B \le Z^{\frac{4}{3}}$ we established the remainder in the total charge $O(Z^{\frac{2}{3}})$. Then using our standard arguments we conclude easily that $|\lambda_N - \nu| = O(Z)$ and then

$$|\lambda_N - \nu| \cdot |\mathsf{N}(\nu) - N| \le CZ^{\frac{5}{3}} \tag{26.3.12}$$

and

$$\mathsf{D}\bigl(P'_B(W_B^{\mathsf{TF}}(x) + \lambda_N) - P'_B(W_B^{\mathsf{TF}}(x) + \nu), \\ P'_B(W_B^{\mathsf{TF}}(x) + \lambda_N) - P'_B(W_B^{\mathsf{TF}}(x) + \nu)\bigr) \le CZ^{\frac{5}{3}}; \tag{26.3.13}$$

combining with the estimate of the previous subsubsection we conclude that

$$\mathsf{D}(\rho_\Psi - \rho_B^{\mathsf{TF}}, \rho_\Psi - \rho_B^{\mathsf{TF}}) \le CQ = O(Z^{\frac{5}{3}}), \tag{26.3.14}$$

exactly as in (25.4.56).

Strong Magnetic Field. Let now $Z^{\frac{4}{3}} \le B \le Z^3$. Then we established the remainder in the total charge $O(Z^{\frac{2}{5}} B^{\frac{1}{5}})$ and for the semiclassical D-term we established estimate $O(Z^{\frac{3}{5}} B^{\frac{4}{5}})$. Therefore to estimate

$$|\lambda_N - \nu| \cdot |\mathsf{N}(\nu) - N| \le CZ^{\frac{3}{5}} B^{\frac{4}{5}} \tag{26.3.15}$$

as well we want to prove that

$$|\lambda_N - \nu| = O(Z^{\frac{1}{5}} B^{\frac{3}{5}}). \tag{26.3.16}$$

Observe that $|\nu| \lesssim Z\bar{r}^{-1} \asymp Z^{\frac{4}{5}} B^{\frac{2}{5}} \le CB$. Therefore if $|\lambda_N - \nu| \le \frac{1}{2}|\nu|$ we conclude that

$$|\int \bigl(P'_B(W_B^{\mathsf{TF}}(x) + \lambda_N) - P'_B(W_B^{\mathsf{TF}}(x) + \nu)\bigr)\, dx| \ge \\ \epsilon|\lambda_N - \nu| B \int (W + \nu)_+^{-\frac{1}{2}}\, dx \tag{26.3.17}$$

with the integral taken over zone $\{x\colon W(x) + \nu \ge |\lambda_N - \nu|\}$.

One can see easily that as $|\lambda_N - \nu| \le \epsilon|\nu|$ the right-hand expression of (26.3.17) is larger than $\epsilon|\lambda_N - \nu| \cdot Z^{\frac{1}{5}} B^{-\frac{2}{5}}$ and it must be less than $CZ^{\frac{2}{5}} B^{\frac{1}{5}}$: $|\lambda_N - \nu| Z^{\frac{1}{5}} B^{-\frac{2}{5}} \le CZ^{\frac{2}{5}} B^{\frac{1}{5}}$ which implies (26.3.16).

Let us estimate the left-hand expression of (26.3.13). For this, however, estimate (26.3.16) is insufficient. We consider here only the atomic case. Then using (26.2.22)–(26.2.23) one can prove easily that the right-hand expression of (26.3.17) is of magnitude

$$|\lambda_N - \nu| \cdot B\bar{r}^2 \times \underbrace{(|\nu|\bar{r}^{-1})^{-\frac{1}{3}} B^{-\frac{1}{3}}} \asymp |\lambda_N - \nu| \cdot |\nu|^{-\frac{1}{3}} Z^{\frac{7}{15}} B^{-\frac{4}{15}}$$

provided $|\lambda - N| \le \epsilon\nu$, where the selected factor is just $\int (B^2 z^4 + |\nu|\bar{r}^{-1})_+^{-\frac{1}{2}}\, dz$ (appearing due to (26.2.22)–(26.2.23)). Comparing with $Z^{\frac{2}{5}} B^{\frac{1}{5}}$ we conclude that

(a) If $|\nu| \ge C_1 Z^{-\frac{1}{10}} B^{\frac{7}{10}}$ $(= C_1 Z^{\frac{2}{5}} B^{\frac{3}{5}} \times Z^{-\frac{3}{10}} B^{\frac{1}{10}})$ then

$$|\lambda_N - \nu| \le C|\nu|^{\frac{1}{3}} Z^{-\frac{1}{15}} B^{\frac{7}{15}} \tag{26.3.18}$$

which is less than $\epsilon|\nu|$ and coincides with (26.3.16) as $(Z - N)_+ \asymp Z$.

(b) If $|\nu| \ge C_1 Z^{-\frac{1}{10}} B^{\frac{7}{10}}$ then $|\lambda_N - \nu| \le C_2 Z^{-\frac{1}{10}} B^{\frac{7}{10}}$.

In the former case one can prove easily that the left-hand expression of (26.3.13) does not exceed $CZ^{\frac{3}{5}} B^{\frac{4}{5}}$.

In the latter case (exactly as in Subsection 25.4.2) we consider Thomas-Fermi theory with $\nu = 0$ i.e. $N = Z$ and also prove that that

(26.3.19) The left-hand expression of (26.3.16) does not exceed $Q = CZ^{\frac{3}{5}} B^{\frac{4}{5}}$.

In particular, we slightly improve estimate (26.3.15) to $|\nu|^{\frac{1}{3}} Z^{\frac{3}{5}} B^{\frac{2}{3}}$ as well (if $(Z - N) \ll Z$).

Therefore in our framework we estimated all non-trace terms in the upper estimate by $CZ^{\frac{3}{5}} B^{\frac{4}{5}}$ and therefore "proved" estimate

$$\mathsf{D}(\rho_\Psi - \rho_B^{\mathsf{TF}}, \rho_\Psi - \rho_B^{\mathsf{TF}}) \le CQ = O(Z^{\frac{3}{5}} B^{\frac{4}{5}}). \tag{26.3.20}$$

Trace

Consider now $\operatorname{Tr}((H_{A,W} - \nu)^-)$. This term is of magnitude $\int (\zeta^5 + B\zeta^3)\, dx$ and one can see easily that it is $\asymp Z^{\frac{7}{3}}$ for $B \le Z^{\frac{4}{3}}$ and $\asymp B^{\frac{2}{5}} Z^{\frac{9}{5}}$ for $Z^{\frac{4}{3}} \le B \le Z^3$.

Meanwhile, consider the remainder. Again for simplicity consider only the atomic case. If $B\le Z$ the contribution of the zone $\{x\colon \ell(x)\le Z^{-\frac{1}{3}}\}$ is $O(Z^{\frac{5}{3}})$ (we need to include Scott correction term in the main part) while the contribution of the zone $\{x\colon \ell(x)\ge Z^{-\frac{1}{3}}\}$ does not exceed

$$C\int (\zeta^3+B\zeta)\ell^{-2}\,dx \tag{26.3.21}$$

taken over this zone and it is $\asymp Z^{\frac{5}{3}}$ as well.

If $Z\le B\le B^2$ the contribution of the zone $\{x\colon \ell(x)\le b:=B^{-\frac{2}{3}}Z^{\frac{1}{3}}\}$ is $O(b^{-\frac{1}{2}}Z^{\frac{3}{2}})=O(Z^{\frac{4}{3}}B^{\frac{1}{3}})$ and we need to include Scott correction term. Meanwhile, the contribution of the zone $\{x\colon \ell(x)\ge b\}$ does not exceed integral (26.3.21) taken over this zone which is $\asymp Z^{\frac{4}{3}}B^{\frac{1}{3}}+Z^{\frac{3}{5}}B^{\frac{4}{5}}$ where the last term coincides with estimate for (26.3.7) if $B\ge Z^{\frac{4}{3}}$ and does not exceed $CZ^{\frac{5}{3}}$ if $B\le Z^{\frac{4}{3}}$.

Finally, if $Z^2\le B\le B^3$ we need to reset $b=Z^{-1}$ because $h=1/(\zeta\ell)$ becomes $\gtrsim 1$ inside. Then we do not need Scott correction term and the contributions of the zone $\{x\colon \ell(x)\le b\}$ to both the main part and the remainder do not exceed $C\int(\zeta^5+B\zeta^3)\,dx\asymp Z^2+B\asymp B$.

Further, the contribution of the zone $\{x\colon \ell(x)\ge b\}$ to the remainder does not exceed integral (26.3.21) taken over this zone which results in $CB+CZ^{\frac{3}{5}}B^{\frac{4}{5}}$ and the second term dominates due to assumption $B\ll Z^3$. Thus we arrive to

(26.3.22) The main therm in $\operatorname{Tr}((H_{A,W}-\nu)^-)$ is of magnitude $Z^{\frac{7}{3}}$ for $B\le Z^{\frac{4}{3}}$ and $B^{\frac{2}{5}}Z^{\frac{9}{5}}$ for $Z^{\frac{4}{3}}\le B\le Z^3$, while the remainder estimate is $O(Z^{\frac{5}{3}})$ for $B\le Z$, $O(Z^{\frac{4}{3}}B^{\frac{1}{3}})$ for $Z\le B\le Z^{\frac{4}{3}}$, and $O(Z^{\frac{4}{3}}B^{\frac{1}{3}}+Z^{\frac{3}{5}}B^{\frac{4}{5}})$ for $Z^{\frac{4}{3}}\le B\le Z^3$.

If $B\le Z^{\frac{7}{4}}$ we need to include into main part Scott correction term.

Discussion

Now let us formulate our expectations:

Remark 26.3.3. We expect

(i) Estimate (26.3.14) for $B\le Z^{\frac{4}{3}}$ and estimate (26.3.20) for $Z^{\frac{4}{3}}\le B\le Z^3$.

(ii) Furthermore, since for $B\le Z^{\frac{4}{3}}$ the main contribution to all terms needed to derive this estimate is delivered by the zone $\{x\colon \ell(x)\approx Z^{-\frac{1}{3}}\}$ and the effective magnetic field is $\mu = B\ell/\zeta \approx BZ^{-1}$ we expect improved to "o" (or better) estimate (26.3.14) if $B \ll Z$ and $a \gg Z^{-\frac{1}{3}}$ [11].

(iii) Statement, similar to (ii) should be also true for the trace term; however then we need to include the Schwinger term.

(iv) The remainder estimate for the ground state energy is maximum of the remainder estimate for the non-trace and trace terms; therefore we expect the same remainder estimate as in (26.3.22); Statement, similar to (ii) should be also correct for the ground state energy. However then we need to include both Schwinger and Dirac terms.

(v) We expect the described remainder estimate of the trace term and the ground state energy if a is large enough; otherwise it should contain term $O(a^{-\frac{1}{2}}Z^{\frac{3}{2}})$ ifs $B \le Z^{\frac{7}{4}}$ and $a \ge Z^{-1}$ (and in this case we include Scott correction term).

Remark 26.3.4. The other difference between cases $B \le Z^{\frac{4}{3}}$ and $B \ge Z^{\frac{4}{3}}$ is that $\mu h = B\zeta^{-2} \lesssim 1$ in the former case if $\ell(x) \le \bar{r}$; however in the latter case it happens only if $\ell(x) \le B^{-1}Z$ but in the zone $\{x\colon B^{-1}Z \le \ell(x) \le B^{-\frac{2}{5}}Z^{\frac{1}{5}}\}$ an opposite inequality holds.

26.3.2 Smooth Approximation

An approach described in Subsection 26.3.1 hits two obstacles: the non-smoothness of W_B^{TF} and its possible degeneration i.e. ∇W_B^{TF} is not disjoint from 0. However non-smoothness of W_B^{TF} is due to the non-smoothness of P_B. So we want to consider first the zone where we can just replace $P_B(W+\nu)$ by $P(W+\nu)$ and therefore W_B^{TF} by some smooth function W which does not necessary coincides with W^{TF}.

Trivial Arguments

Obviously we can do this as an effective magnetic field $\mu = B\ell/\zeta \lesssim 1$. In this case we do not need assumption $W + \nu \asymp \zeta^2$ and therefore we can take $\zeta = \ell^{-4}$ as $B \lesssim Z^{\frac{4}{3}}$ and $\ell \gtrsim Z^{-\frac{1}{3}}$ <u>and</u> $\zeta = Z^{\frac{1}{2}}\ell^{-\frac{1}{2}}$ in all other cases. Therefore zone in question is

[11] Recall that $a = \min_{1\le m<m'\le M} |\mathsf{y}_m - \mathsf{y}_{m'}|$ is the minimal distance between nuclei.

$$\mathcal{X}_1 := \{x\colon \ell(x) \le r_1\} \quad \text{with} \quad r_1 = \begin{cases} B^{-\frac{1}{3}} & \text{if } 1 \le B \lesssim Z, \\ B^{-\frac{2}{3}} Z^{\frac{1}{3}} & \text{if } Z \lesssim B \lesssim Z^2. \end{cases} \tag{26.3.23}$$

In this zone $\mathcal{X}_1$ for such modified W we can unleash the full power of the same smooth theory as in Section 25.4 and prove easily the following

Proposition 26.3.5. *Let* $1 \le B \le Z^2$. *Then*

(i) A contribution of zone $\mathcal{X}_1$ *defined by* (26.3.23) *to*

$$\int \Bigl(e(x,x,\nu) - P'(W(x)+\nu)\Bigr)\, dx \tag{26.3.24}$$

does not exceed $CZ^{\frac{2}{3}}$ *while its contribution to*

$$\mathsf{D}\Bigl(e(x,x,\nu) - P'(W(x)+\nu), e(x,x,\nu) - P'(W(x)+\nu)\Bigr) \tag{26.3.25}$$

does not exceed $CZ^{\frac{5}{3}}$, *and its contribution to*

$$\int \Bigl(e_1(x,x,\nu) + P(W(x)+\nu)\Bigr)\, dx - \mathsf{Scott} \tag{26.3.26}$$

does not exceed $CZ^{\frac{5}{3}} + Ca^{-\frac{1}{2}}Z^{\frac{3}{2}} + CZ^{\frac{4}{3}}B^{\frac{1}{3}}$ [11], [12].

(ii) Further, if $B \ll Z$ *and* $a \gg Z^{-\frac{1}{3}}$ *we can recover for these contributions estimates* $CZ^{\frac{2}{3}}\upsilon$, $CZ^{\frac{5}{3}}\upsilon$ *and* $CZ^{\frac{5}{3}}\upsilon$ *respectively with*

$$\upsilon := Z^{-\delta} + (aZ^{\frac{1}{3}})^{-\delta} + (BZ^{-1})^{\delta} \tag{26.3.27}$$

where expression (26.3.26) *should be modified to*

$$\int \bigl(e_1(x,x,\nu) - P(W(x)+\nu)\bigr)\, dx - \mathsf{Scott} - \mathsf{Schwinger}. \tag{26.3.28}$$

Furthermore in this case contribution of $\mathcal{X}_1$ *to*

$$\frac{1}{2}\int \mathrm{tr}\bigl(e^{\dagger}(x,y,\nu)e(x,y,\nu)\bigr)\, dxdy - \mathsf{Dirac} \tag{26.3.29}$$

does not exceed $CZ^{\frac{5}{3}-\delta}$.

[12] If $a \lesssim Z^{-1}$ we skip Scott and reset $a = Z^{-1}$ in the remainder estimate which become CZ^2.

Remark 26.3.6. (i) So far we should use $P(.)$ instead of $P_B(.)$ but we will prove that the same results would hold for P_B as well.

(ii) In the next subsubsections we expand this zone to one defined by $\mu \le h^{-\frac{1}{3}}$ [13)] but for trace term we still need a separate analysis as $\mu \lesssim 1$.

(iii) The same estimates hold if we replace in all expressions (26.3.24)–(26.3.28) P by P_B.

(iv) We assumed that $B \le Z^2$ since otherwise $h \gtrsim 1$ not only in $\mathcal{X}_1$ but even in $\{x\colon W^{\mathsf{TF}}(x) \ge B\}$.

(v) Note that if $r_1 \gtrsim (Z-N)_+^{-\frac{1}{3}}$ this zone (and the whole analysis) could be cut short since outside zone in question $W + \nu \ge 0$. From Chapter 25 we already know how to deal with such irregularities.

(vi) We need to assume that $a \ge Z^{-\frac{1}{3}}$ and to include the second term $(aZ^{\frac{1}{3}})^{-\delta}$ in the definition of υ only as we estimate the trace term (26.3.26).

Remark 26.3.7. (i) If either $a \ll Z^{-\frac{1}{3}}$ or $B \gg Z$ we estimated (26.3.5) by $Ca^{-\frac{1}{2}}Z^{\frac{3}{2}} + CZ^{\frac{4}{3}}B^{\frac{1}{3}}$. While the first term does not bother us since assumption $a \ll \min(Z^{-\frac{1}{3}}, B^{-\frac{1}{4}})$ is unrealistic, the second term is troublesome. Let us assume that $a \ge Z^{-\frac{1}{3}}$.

We can marginally improve this estimate of expression (26.3.26) to $CZ^{\frac{5}{3}} + o\bigl(Z^{\frac{4}{3}}B^{\frac{1}{3}}\bigr)$.

First, observe, that this term $CZ^{\frac{3}{2}}B^{\frac{1}{3}}$ appears as $b^{-\frac{1}{2}}Z^{\frac{3}{2}}$ with $b = B^{-\frac{2}{3}}Z^{\frac{2}{3}} \ll 1$. Therefore we need to estimate this way only contribution of the zone $\mathcal{Y} := \{x\colon b^{\delta} \le \ell(x)Z^{\frac{1}{3}} \le b^{-\delta}\}$ and it is sufficient to investigate the corresponding classical dynamics in the zone $\mathcal{Y}_1 := \{x\colon b^{2\delta} \le \ell(x)Z^{\frac{1}{3}} \le b^{-2\delta}\}$.

Indeed, to recover estimate we have now, we used a classical dynamics on $\Sigma := \{(x,\xi)\colon H(x,\xi) = 0\}$ for time $T(x) = Z^{-1}\ell(x)^{\frac{3}{2}}$.

Further, one can see easily that along classical trajectories, starting in $\Sigma|_{\mathcal{Y}}$, $\ell(x) \le b^{-2\delta}$ for time $T = b^{-\sigma}T_0$ with $\sigma = \sigma(\delta) > 0$.

On the other hand, the invariant measure of $\Sigma_r = \{(x,\xi) \in \Sigma, \ell(x) \asymp r\}$ is $\asymp r^2 Z$ and since the spatial speed there is $O(Z^{\frac{1}{2}}r^{-\frac{1}{2}})$ we conclude that

13) Or even to $\mu \le h^{-\frac{3}{5}}$ under non-degeneracy assumption (26.3.35) with $\gamma = \ell$, in particular, in the atomic case.

(26.3.30) The invariant measure of the points in $\Sigma|_{\mathcal{Y}}$, such that the classical trajectories starting from them do not remain in $\mathcal{Y}_1$ for time $T = b^{-\sigma}T_0$, does not exceed $b^{2+\sigma}Z^{\frac{1}{3}}$.

(ii) Now it is sufficient to explore the classical dynamics with the Hamiltonian, corresponding to the Coulomb potential and constant magnetic field, and to prove that

(26.3.31) The invariant measure of the periodic points Σ is 0.

To do so, we need to prove that there are non-periodic trajectories, which do not hit an origin. It is sufficient to consider trajectories belonging to the plane $\{z = 0\}$; we assume that magnetic intensity is $(0, 0, B)$. See Part (iii).

(iii) To improve this estimate further we need to investigate the classical dynamics in more details, and it seems to be a daunting, if not impossible task. Indeed, while in 2D the system is completely integrable[14)], it does not seem so in 3D as we know only two first integrals, energy E and $M_z = (x\dot{y} - y\dot{x}) + \frac{1}{2}B(x^2 + y^2)$.

Formal Expansion

Now we want to expand zone $\mathcal{X}_1$. Note first that

$$P'_B(W + \nu) - P'(W + \nu) = O(B^{\frac{3}{2}}) \tag{26.3.32}$$

and

$$P_B(W + \nu) - P(W + \nu) - \kappa_1 B^2(W + \nu)^{\frac{1}{2}} = O(B^{\frac{5}{2}}). \tag{26.3.33}$$

Really, one can consider $P'_B(w)$ and $P_B(w)$ as Riemann sums for integrals $P'(w)$ and $P(w)$ respectively; see Appendix 26.A.3 for details.

However under non-degeneracy assumption $|\nabla W| \asymp \zeta^2\ell^{-1}$ we can do better with the integrated expressions.

[14)] And easily solvable in the polar coordinates since $E = \frac{1}{2}\dot{r}^2 + V^*(r)$ with effective potential $V^*(r) = \frac{1}{2}r^2(M_z r^{-2} - B/2)^2 - r^{-1}$, and the corrected angular momentum $M_z = r^2\dot{\theta} + \frac{1}{2}Br^2$. One can see easily that $V^*(r) \to +\infty$ as $r \to +0$ or $r \to +\infty$ and has a single nondegenerate minimum. Therefore along each trajectory r oscillates between $r_{\min}$ and $r_{\max}$. If all trajectories on the energy level E were periodic, then the number of oscillations was constant for increment θ equal to $2\pi n$ with some $n \in \mathbb{Z}^+$. But this is definitely not the case since the number of oscillations tends to ∞ as $M_z/B \to +\infty$.

Proposition 26.3.8. *Assume that in* $B(z,\gamma)$

$$|\nabla^\alpha W|\le C_\alpha \zeta^2\gamma^{-|\alpha|}\qquad \forall \alpha: |\alpha|\le n, \tag{26.3.34}$$

$$|\nabla W|\ge \epsilon\zeta^2\gamma^{-1}, \tag{26.3.35}$$

and

$$B\le \zeta^2. \tag{26.3.36}$$

Then

$$\int \phi(x)\Bigl(P'_B(W(x)+\nu)-\tilde{P}'_B(W(x)+\nu)\Bigr)\,dx = O(B^2\zeta^{-1}\gamma^3), \tag{26.3.37}$$

$$\int \phi(x)\Bigl(P_B(W(x)+\nu)-\tilde{P}'_B(W(x)+\nu)\Bigr)\,dx = O(B^5\zeta^{-5}\gamma^3) \tag{26.3.38}$$

and

$$\begin{multline}\mathsf{D}\Bigl(\phi(x)\bigl(P'_B(W(x)+\nu)-\tilde{P}'_B(W(x)+\nu)\bigr),\\ \phi(x)\bigl(P'_B(W(x)+\nu)-\tilde{P}'_B(W(x)+\nu)\bigr)\Bigr) = O(B^5\zeta^{-4}\gamma^5)\end{multline} \tag{26.3.39}$$

with

$$\tilde{P}_B(w) \coloneqq P(w) + \bigl(\kappa_1 P''(w)B^2 + \kappa_2 P^{IV} B^4\bigr)\cdot\bigl(1-\varphi(w/B)\bigr) \tag{26.3.40}$$

where $\varphi\in\mathscr{C}^\infty([-2,2])$, $\varphi=1$ *on* $[-1,1]$.

Proof. Rescaling $x\mapsto x\gamma^{-1}$, $w\mapsto w\zeta^{-2}$ and therefore $B\mapsto \beta = B\zeta^{-2}$ one can reduce the case to $\gamma=\zeta=1$, $\beta\le 1$ [15]. Then estimates (26.3.37) and (26.3.38) are trivially proven by (multiple) integration by parts which integrates P_β on each step increasing its smoothness[16].

To prove estimate (26.3.39) we apply decomposition (26.3.8). Integration by parts shows that (26.3.37) with t-admissible function ϕ is $O(\beta^3 t^{\frac{3}{2}})$ if $t\ge\beta$ and therefore the contribution of the zone $\{(x,y)\colon |x-y|\asymp t\}$ is $O(\beta^6 t^3\times t^{-4})$. Then the total contribution of the zone $\{(x,y)\colon |x-y|\ge\beta\}$ is $O(\beta^5)$. Meanwhile a total contribution of the zone $\{(x,y)\colon |x-y|\le\beta\}$ is $O(\beta^3\times\beta^2)$.

[15] Recall that $\beta=\mu h$ with $\mu=B\gamma/\zeta$ and $h=1/\zeta\gamma$.

[16] In fact one can prove then estimates $O(\beta^s)$ but adding correction terms $\sum\kappa_k\beta^{2k}$. However this improvement is not carried on to (26.3.39) in full.

Therefore we expect that the zone $\mathcal{X}_1$ defined by $\mu \lesssim 1$ could be expanded to the zone $\mathcal{X}'_1$ defined by $\mu \lesssim h^{-\frac{1}{3}}$ [13] or even larger[17]; furthermore, under assumption $|\nabla W| \asymp \zeta^2\ell^{-1}$ we can define $\mathcal{X}'_1$ by $\mu \lesssim h^{-\frac{3}{5}}$ or even larger[17].

Expansion: Justification

Now however we need to deal with $e(x,x,\nu)$ rather than $P'_B(W(x)+\nu)$ (etc).

Proposition 26.3.9. *Assume that in* $B(z,\gamma)$ *conditions* (26.3.34), $\zeta\gamma \ge 1$ *and*

$$B \le c\zeta^2(\zeta\gamma)^{-\delta} \tag{26.3.41}$$

are fulfilled. Then for γ*-admissible* ϕ

$$\int \phi(x)\Bigl(e(x,x,\nu) - \tilde{P}'_B(W(x)+\nu)\Bigr)\,dx = O(\zeta^2\gamma^2), \tag{26.3.42}$$

$$\int \phi(x)\Bigl(e_1(x,x,\tau) - \tilde{P}_B(W(x)+\nu)\Bigr)\,dx = O(\zeta^3\gamma) \tag{26.3.43}$$

and

$$\begin{aligned}\mathsf{D}\Bigl(\phi(x)\bigl(e(x,x,\nu) - \tilde{P}'_B(W(x)+\nu)\bigr),&\\ \phi(x)\bigl(e(x,x,\nu) - \tilde{P}'_B(W(x)+\nu)\bigr)\Bigr) &= O(\zeta^4\gamma^3).\end{aligned} \tag{26.3.44}$$

Proof. Estimates (26.3.42) and (26.3.43) are due to Chapter 13. Really, rescale $x \mapsto x\gamma^{-1}$, $\tau \mapsto \tau\zeta^{-2}$ and $h=1 \mapsto h=\gamma^{-1}\zeta^{-1}$, $B \mapsto \mu = B\gamma\zeta^{-1}$.

To prove (26.3.44) let us apply decomposition (26.3.8); then according to (26.3.42) $J(t)$ (defined as expression (26.3.42) with $t\gamma$-admissible ϕ_t) does not exceed $C\zeta^2\gamma^2t^2$ as long as $t\zeta\gamma \ge 1$; therefore contribution of zone $\{(x,y)\colon |x-y| \asymp t\}$ into the left-hand expression of (26.3.44) does not exceed $C(\zeta^2\gamma^2t^2)^2 \times t^{-4}\gamma^{-1} \asymp C\zeta^4\gamma^3$.

Then summation over $t \ge \mu^{-1} = B^{-1}\gamma^{-1}\zeta$ returns $C\zeta^4\gamma^3\int t^{-1}\,dt \asymp C\zeta^4\gamma^3\log\mu$ (we assume that $\mu \ge 2$; case $\mu \lesssim 2$ has been covered already). So, the total contribution of zone $\{(x,y)\colon |x-y| \ge \mu^{-1}\}$ does not exceed $C\zeta^4\gamma^3\log\mu$.

[17] We do not need for each ℓ have a sharp remainder estimates but need only them to sum to a sharp estimate.

Let us get rid of the logarithmic factor. Returning back to $B(z,t)$ stretched to $B(0,1)$ one can see easily that conditions of Proposition 13.7.25 are fulfilled as well with $T = \min\bigl(t^{-\delta}, h^{-\delta}t^{\delta}\bigr)$ and thus

$$|J(t)| \le C(ht^{-1})^{-2}T^{-1} \le Ch^{-2}t^2\bigl(t^{\delta} + h^{\delta}t^{-\delta}\bigr).$$

Plugginginto (26.3.8) we get

$$Ch^{-4}\gamma^{-1}\int_{\mu^{-1}}^{1} t^{-1}\bigl(t^{\delta} + h^{\delta}t^{-\delta}\bigr)\,dt \asymp Ch^{-4}\gamma^{-1} = C\zeta^4\gamma^3.$$

On the other hand, in zone $t \le \mu^{-1}$ we use the trivial estimate

$$e(x,x,\nu) - P'(W(x)+\nu) = O(\mu\zeta^2\gamma^2)$$

(due to simple rescaling $x \mapsto \mu x$) and its contribution to the left-hand expression of (26.3.44) does not exceed $C(\mu\zeta^2\gamma^2)^2 \times \mu^{-2}\gamma^{-1} \asymp C\zeta^4\gamma^3$. □

Combining with estimates (26.3.32) and (26.3.33) we arrive to Statement (i) below; combining with Proposition 26.3.7 to Statement (ii):

Corollary 26.3.10. *Assume that in $B(z,\gamma)$ conditions (26.3.34) and $\zeta\gamma \ge 1$ are fulfilled. Let ϕ be γ-admissible function.*

(i) Let

$$B \le c\zeta^{\frac{4}{3}}\gamma^{-\frac{2}{3}}; \tag{26.3.45}$$

then

$$\int \phi(x)\Bigl(e(x,x,\nu) - \tilde{P}'_B(W(x)+\nu)\Bigr)\,dx = O(\zeta^2\gamma^2), \tag{26.3.46}$$

$$\int \phi(x)\Bigl(e_1(x,x,\tau) - \tilde{P}_B(W(x)+\nu)\Bigr)\,dx = O(\zeta^3\gamma) \tag{26.3.47}$$

and

$$\begin{aligned}\mathsf{D}\Bigl(\phi(x)\bigl(e(x,x,\nu) - \tilde{P}'_B(W(x)+\nu)\bigr),&\\ \phi(x)\bigl(e(x,x,\nu) - \tilde{P}'_B(W(x)+\nu)\bigr)\Bigr) &= O(\zeta^4\gamma^3).\end{aligned} \tag{26.3.48}$$

(ii) Let assumption (26.3.35) be fulfilled and

$$B \le c\zeta^{\frac{8}{5}}\gamma^{-\frac{2}{5}}. \tag{26.3.49}$$

Then (26.3.46)–(26.3.48) hold.

26.3.3 Rough Approximation

Unless our analysis has been cut short with $r_1 \gtrsim (Z-N)_+^{-\frac{1}{3}}$, we need to consider the zone $\{x\colon \ell(x)\ge r_1\}$ with redefined r_1, so that this zone is described by $\mu \gtrsim h^{-\frac{1}{3}}$ or $\mu \gtrsim h^{-\frac{3}{5}}$ in the general or non-degenerate (i.e. satisfying assumption (26.3.35)) cases respectively.

In this zone the replacement of P_B by P and thus W_B^{TF} by some smooth function leads to the error which is too large. Therefore instead in this zone we consider $\varepsilon\ell$-mollification of W_B^{TF} with $\varepsilon \ll 1$ (after rescaling $x\mapsto x/\ell$). In contrast to potentials considered in Chapter 18 function W_B^{TF} is more regular.

Properties of Mollification

First, recall regularity properties of W_B^{TF}:

Proposition 26.3.11. W_B^{TF} *have the following properties:*

$$|\nabla^\alpha W_B^{\mathsf{TF}}(x)| \le c_\alpha \zeta(x)^2\ell(x)^{-|\alpha|} \qquad \forall \alpha : |\alpha|\le 2, \tag{26.3.50}$$

$$\begin{aligned}|\nabla^\alpha \bigl(W_B^{\mathsf{TF}}(x)-W_B^{\mathsf{TF}}(y)\bigr)| \le\\ c_0B\ell(x)^{-\frac{5}{2}}|x-y|^{\frac{1}{2}} + c_0\zeta(x)^2\ell(x)^{-3}|x-y|\\ \forall |\alpha|=2 \quad \forall x,y\colon |x-y|\le \epsilon\ell(x)\end{aligned} \tag{26.3.51}$$

where we recall

$$\zeta(x)=\min\bigl(Z^{\frac{1}{2}}\ell(x)^{-\frac{1}{2}}, \ell(x)^{-2}\bigr) \qquad \textit{if}\ \ B\le Z^{\frac{4}{3}}, \tag{26.3.52}$$

$$\zeta(x)=Z^{\frac{1}{2}}\ell(x)^{-\frac{1}{2}} \qquad \textit{if}\ \ B\ge Z^{\frac{4}{3}}; \tag{26.3.53}$$

Proof. This proof is rather obvious corollary of the Thomas-Fermi equation (26.2.3). See also arguments below. □

Let us consider $B(z,\ell(z))$ with $\zeta^2\gtrsim B$ and rescale $x\mapsto x\ell^{-1}$, $W\mapsto w=\zeta^{-2}(W+\nu)$ (where we included ν for a convenience). After such rescaling $w\in\mathscr{C}^{\frac{5}{2}}$ uniformly, but there is more: Thomas-Fermi equation (26.2.3) translates into

$$\frac{1}{4\pi}\Delta w = \ell^2P'_\beta(w) = \ell^2\zeta P'(w) + \ell^2\zeta\bigl(P'_\beta(w)-P'(w)\bigr) \tag{26.3.54}$$

with $\beta = B\zeta^{-2}$; observe that $P'_B(W)$ is positively homogeneous of degree 3 with respect to (W,B).

Note that parameter $\eta := \zeta\ell^2 \lesssim 1$ and $\eta \asymp 1$ if and only if $B \lesssim Z^{\frac{4}{3}}$ and $\ell \gtrsim Z^{-\frac{4}{3}}$ (in which case $\zeta \asymp \ell^{-2}$).

Also note that the first term and the second terms in the right-hand expression of (26.3.54) belong to $\mathscr{C}^{\frac{5}{2}}$ and $\beta\eta\mathscr{C}^{\frac{1}{2}}$ respectively uniformly[18] and

$$\beta\eta = \beta\zeta\ell^2 = B\zeta^{-1}\ell^2, \qquad \eta := \zeta\ell^2 \qquad \text{if } \beta \lesssim 1. \tag{26.3.55}$$

Because of this $w \in \mathscr{C}^{\frac{9}{2}} \oplus \beta\eta\mathscr{C}^{\frac{5}{2}}$ again uniformly. Iterating, we conclude that $w \in \mathscr{C}^n \oplus \beta\eta\mathscr{C}^{\frac{5}{2}}$ with arbitrarily large exponent n.

On the other hand, if $B \gtrsim \zeta^2$ (i.e. $\beta \gtrsim 1$) without invoking P'_B one can prove easily that $w \in \eta\mathscr{C}^{\frac{5}{2}}$ with

$$\eta := \beta\zeta\ell^2 = B\zeta^{-1}\ell^2 \qquad \text{if } \beta \gtrsim 1. \tag{26.3.55$'$}$$

Therefore we have proven

(26.3.56) $w \in \mathscr{C}^n \oplus \beta\eta\mathscr{C}^{\frac{5}{2}}$ with arbitrarily large exponent n as $\beta \lesssim 1$ and $w \in \eta\mathscr{C}^{\frac{5}{2}}$ as $\beta \gtrsim 1$

and one can see easily that

(26.3.57) Parameter $\eta = B\zeta^{-1}\ell^2$ is $O(1)$ and $\eta \asymp 1$ iff either $B \le Z^{\frac{4}{3}}$ and $\ell \asymp B^{-\frac{1}{4}}$ or $B \ge Z^{\frac{4}{3}}$ and $\ell \asymp B^{-\frac{2}{5}}Z^{\frac{1}{5}}$ (i.e. near border of $\mathsf{supp}(\rho_B^{\mathsf{TF}})$, uncut by ν).

Remark 26.3.12. It may seem strange to define η differently as $\beta \lesssim 1$ and $\beta \gtrsim 1$ but there is a good reason for this when we consider the case of $M \ge 2$. Anyway, η is the magnitude of the right-hand expression of (26.3.54).

Proposition 26.3.13. *(i) Let w_ε be a ε-mollification of w with $\varepsilon \lesssim \min(\beta, h^\delta)$ (recall that $h = 1/(\zeta\ell)$). Then if $\beta \lesssim 1$ the following estimates hold:*

$$|\nabla^\alpha (w - w_\varepsilon)| \le c_\alpha \beta\eta\varepsilon^{\frac{5}{2}-|\alpha|} \qquad \forall \alpha : |\alpha| \le 2, \tag{26.3.58}$$

$$|P_\beta(w) - P_\beta(w_\varepsilon)| \le c\beta\eta\varepsilon^{\frac{5}{2}} \tag{26.3.59}$$

and

$$|P'_\beta(w) - P'_\beta(w_\varepsilon)| \le c\beta^{\frac{3}{2}}\eta^{\frac{1}{2}}\varepsilon^{\frac{5}{4}} + c\beta\eta\varepsilon^{\frac{5}{2}}; \tag{26.3.60}$$

[18] I.e. norms do not depend on any parameters.

(ii) On the other hand, if $\beta \gtrsim 1$ the right-hand expressions of (26.3.58)–(26.3.60) *should be replaced by the similar expressions albeit without β:*

$$|\nabla^\alpha(w - w_\varepsilon)| \le c_\alpha \eta \varepsilon^{\frac{5}{2}-|\alpha|} \qquad \forall \alpha : |\alpha| \le 2, \tag{26.3.58$'$}$$

$$|P_\beta(w) - P_\beta(w_\varepsilon)| \le c\eta\varepsilon^{\frac{5}{2}} \tag{26.3.59$'$}$$

and

$$|P'_\beta(w) - P'_\beta(w_\varepsilon)| \le c\eta^{\frac{1}{2}}\varepsilon^{\frac{5}{4}}. \tag{26.3.60$'$}$$

(iii) Further, under assumption $|\nabla w| \asymp 1$ in both cases

$$|\int \phi(x)\bigl(P_\beta(w) - P_\beta(w_\varepsilon)\bigr)\, dx| \le c\eta\varepsilon^{\frac{7}{2}}, \tag{26.3.61}$$

$$|\int \phi(x)\bigl(P'_\beta(w) - P'_\beta(w_\varepsilon)\bigr)\, dx| \le c\eta\varepsilon^{\frac{9}{4}} \tag{26.3.62}$$

and

$$\mathsf{D}\bigl(\phi(P'_\beta(w) - P'_\beta(w_\varepsilon)),\, \phi(P'_\beta(w) - P'_\beta(w_\varepsilon))\bigr) \le c\eta^2\varepsilon^{\frac{9}{2}}. \tag{26.3.63}$$

Proof. Proof of Statement (i) is trivial; in particular, we observe that $\eta\varepsilon^{\frac{5}{2}} \lesssim \beta$.

Proof of Statement (iii) is also easy since then w_ε is different from w on the set of measure $\asymp \beta^{-1}\varepsilon$ if $\beta \le C_0$ and on the set of measure $\asymp \varepsilon$ if $\beta \ge C_0$. Actually w is uniformly smooth if $\beta \gtrsim 1$ and $\ell(x) \le \epsilon\bar{r}$ and we do not need any mollification here.

One definitely can improve estimates (26.3.61)–(26.3.63) but we do not need it. □

Consider now the analytical expressions and estimate the semiclassical errors.

Remark 26.3.14. (i) From now on until the end of this Section we assume that $M = 1$ to avoid possible degenerations.

(ii) Recall that we can reduce operator with mollified potential to a canonical form provided $\varepsilon \ge C(\mu^{-1}h)^{\frac{1}{2}}|\log\mu|$ (see Section 18.7). However here we will have a much better estimate since we will take $\varepsilon \ge h^{\frac{2}{3}-\delta}$.

Charge Term

Let us consider the *charge term* i.e. expression $\int e(x,x,\nu)\, dx = (\operatorname{Tr}\theta(\nu - H))$.

Regular Zone. Then the results of Section 18.9 implies that as

$$W + \nu \asymp \zeta^2 \tag{26.3.64}$$

and

$$|\nabla W| \asymp \zeta^2 \ell^{-1} \tag{26.3.65}$$

contribution of the ball $B(x, \ell(x))$ to expression (26.3.24) does not exceed $C(1 + \mu h)h^{-2} \asymp C\zeta^2\ell^2 + CB\ell^2$ exactly as in the mock proof.

Then summation with respect to ℓ-partition in this zone results in $CB^{\frac{2}{3}}$ as $B \le Z$, $CZ^{\frac{2}{3}}$ as $Z \le B \le Z^{\frac{4}{3}}$ and $CB^{\frac{1}{5}}Z^{\frac{2}{5}}$ as $Z^{\frac{4}{3}} \le B \le Z^3$.

Remark 26.3.15. (i) Condition (26.3.64) is fulfilled as $\ell(x) \le \epsilon \bar{r}$.

(ii) Further, since $M = 1$ both conditions (26.3.64) and (26.3.65) are fulfilled if $|x| \le (1 - \epsilon)\bar{r}_m$ (we pick up $\mathsf{y}_m = 0$ and $\bar{r}_m$ exact radius of $\mathsf{supp}(\rho_B^{\mathsf{TF}})$).

Border Strip. Now we need to consider the contribution of the border strip $\mathcal{Y} := \{x : \gamma(x) \le \epsilon\}$ with $\gamma(x) = \epsilon(\bar{r} - |x|)\bar{r}^{-1}$ and $\bar{r} := \bar{r}_m$. Here $\ell \asymp \bar{r}$, $\zeta \asymp \bar{\zeta}$ with

$$\bar{r} \asymp \begin{cases} (Z - N)_+^{-\frac{1}{3}} & \text{if } B \le (Z - N)_+^{\frac{4}{3}}, \\ B^{-\frac{1}{4}} & \text{if } (Z - N)_+^{\frac{4}{3}} \le B \le Z^{\frac{4}{3}}, \\ Z^{\frac{1}{5}} B^{-\frac{2}{5}} & \text{if } Z^{\frac{4}{3}} \le B \le CZ^3 \end{cases} \tag{26.3.66}$$

and

$$\bar{\zeta} \asymp \begin{cases} (Z - N)_+^{\frac{2}{3}} & \text{if } B \le (Z - N)_+^{\frac{4}{3}}, \\ B^{\frac{1}{2}} & \text{if } (Z - N)_+^{\frac{4}{3}} \le B \le Z^{\frac{4}{3}}, \\ Z^{\frac{2}{5}} B^{\frac{1}{5}} & \text{if } Z^{\frac{4}{3}} \le B \le CZ^3 \end{cases} \tag{26.3.67}$$

and scaling we get $\mu = B\bar{r}\bar{\zeta}^{-1}$ and $h = \bar{\zeta}^{-1}\bar{r}^{-1}$ here.

Let us consider first the case $\nu = 0$. Then both conditions (26.3.64) and (26.3.65) are fulfilled albeit with $\ell_1 = \gamma(x)\bar{r}$ and $\varsigma(x) = \bar{\zeta}\gamma(x)^2$ instead of ℓ and ζ.

Thus if $\varsigma\ell_1 \ge 1$ (i.e. $\gamma \ge \bar{\gamma} := h^{\frac{1}{3}}$), the contribution of the ball $B(x, \gamma(x)\bar{r})$ to the remainder does not exceed $C\mu h^{-1}\gamma^2$ [19] and therefore the total contribution of zone $\mathcal{Y}_1 := \{x : \bar{\gamma} \le \gamma(x) \le \epsilon\bar{r}\}$ to the remainder does not

[19] Really, after additional rescaling $x \mapsto x\gamma^{-1}$, $w \mapsto w\gamma^{-2}$ we have $\mu_1 = \mu\gamma^{-1}$, $h_1 = h\gamma^{-3}$ and $\mu_1 h_1^{-1} = \mu h^{-1}\gamma^2$.

exceed

$$C\mu h^{-1}\int \gamma(x)^{-1}\,dx \asymp C\mu h^{-1}|\log h| = CB\bar{r}^2|\log h| \tag{26.3.68}$$

which is $O(Z^{\frac{2}{3}})$ as long as $B\le Z^{\frac{4}{3}}(\log Z)^{-2}$.

Further, the same approach works if $|\nu|\lesssim \bar{\zeta}^2\bar{\gamma}^3\asymp \bar{\zeta}^2 h\asymp \bar{\zeta}\bar{r}^{-1}$ which is equivalent to $(Z-N)_+\le \bar{\zeta}$ (then $|\nabla W|\asymp \varsigma^2\ell_1^{-1}$ if $\gamma(x)\ge\bar{\gamma}$) <u>and</u> also if this condition is violated but $|\nu|\le\bar{\zeta}^2$; in the latter case we need to pick up $\bar{\gamma}=\bar{\gamma}_1:=|\nu|^{\frac{1}{3}}\bar{\zeta}^{-\frac{2}{3}}$.

To get rid of the logarithmic factor let us consider propagation. Recall that it goes along magnetic lines i.e. that (x_1,x_2) remains constant. Let us consider propagation in the direction in which $|x_3|$ increases (i.e. $\gamma(x)$ decays); we do not need to consider zone $\mathcal{Y}_1\cap\{|x_3|\le Z^{-\delta}\bar{r}\}$ since contribution of this zone (26.3.68) is $o(B\bar{r}^2)$.

One can see easily that we can follow dynamics which does not return for a time $T_1^*(x):=T_1(x)(\gamma(x)/\bar{\gamma})^\delta$ where $T(x)\asymp \ell_1^{-1}\varsigma^{-1}\asymp \bar{r}\bar{\zeta}^{-1}\gamma^{-1}$ is a time required for this dynamics to pass though $B(x,\ell_1(x))$. Therefore one can replace (26.3.68) by

$$C\mu h^{-1}\int_{\{x:\,\gamma(x)\ge\bar{\gamma}\}}\bar{\gamma}^\delta\gamma(x)^{-1-\delta}\,dx\asymp C\mu h^{-1}=CB\bar{r}^2. \tag{26.3.69}$$

Further, as $|\nu|\ge B\bar{r}$ we need also to consider zone $\mathcal{Y}_0:=\{x\colon \gamma(x)\le\bar{\gamma}\}$. In this zone we take $\ell_1=\bar{\ell}_1=\bar{\gamma}\bar{r}$ and $\varsigma=\bar{\varsigma}=(|\nu|\bar{\gamma})^{\frac{1}{2}}$ with $\ell_1\varsigma\ge 1$ and since $|\nabla W|\asymp\varsigma^2\ell_1^{-1}$, contribution of $B(x,\ell_1(x))$ to the remainder does not exceed $CB\bar{\ell}_1^2$ and the total contribution of $\mathcal{Y}_2$ does not exceed $CB\bar{r}^2$ which what exactly we achieved for zone $\mathcal{Y}_1$ after we got rid of logarithm. We take mollification parameter $\varepsilon=\bar{\varsigma}^{-1}Z^{\delta}$[20].

Furthermore, zone $\mathcal{Y}_3=\{x\colon |x|\ge\bar{r}+\bar{\ell}_1\}$ is classically forbidden. So we can take here

$$\ell_1(x)=\epsilon(|x|-\bar{r}),\qquad \varsigma(x)=\min\bigl(\bar{\varsigma}\bar{\ell}_1^{-\frac{1}{2}}\ell_1(x)^{\frac{1}{2}},|\nu|^{\frac{1}{2}}\bigr) \tag{26.3.70}$$

and prove easily that its contribution also does not exceed $CB\bar{r}^2$.

Returning to the case $|\nu|\lesssim\bar{\zeta}$ we see that the contribution of zone $\mathcal{Y}_2$ to the remainder does not exceed $CB\bar{r}^2$ because effective semiclassical

[20] One can see easily that the resulting errors in the expressions(26.3.24) and (26.3.25)–(26.3.26) will not violate our claims.

parameter here is $h_1 = 1$ and non-degeneracy condition is of no concern for us. We take mollification parameter $\varepsilon = \bar{\varsigma}^{-1} Z^{\delta}$[20].

Moreover, we can modify W in $\mathcal{Y}_2$ (make it negative there) so that this zone would be classically forbidden with ℓ_1, ς defined by (26.3.70) with $|\nu|$ replaced by $\bar{\zeta}$.

Finally in the case $B \le |\nu|$ (i. e. $B \le C(Z-N)_+^{\frac{4}{3}}$ we can apply the above arguments with $\bar{\gamma} = 1$ and arrive to the same result. Therefore we proved in all cases

(26.3.71) If $M = 1$ the total contribution of the border strip $\mathcal{Y}$ to the remainder in the charge term is $O(B\bar{r}^2)$ which does not exceed $CB^{\frac{1}{2}}$ as $B \le Z^{\frac{4}{3}}$ and $CB^{\frac{1}{5}} Z^{\frac{2}{5}}$ if $Z^{\frac{4}{3}} \le B \le Z^3$.

Conclusion. If $Z^2 \le B \le Z^3$ we need to estimate also contribution of the *inner core* $\mathcal{X}_0 := \{x\colon \ell(x) \le CZ^{-1}\}$. By means of variational methods we will prove (see Corollary 26.A.5)

(26.3.72) If $Z^2 \le B \le Z^3$ the contributions of $\mathcal{X}_0$ to both $\int e(x,x,\nu)\,dx$ and $\int P'_B(W(x)+\nu)\,dx$ do not exceed CBZ^{-2}.

Then we arrive to the following

Proposition 26.3.16. *Let $M = 1$. Then*

(i) For constructed above potential W expression (26.3.24) *does not exceed $CZ^{\frac{2}{3}} + CB^{\frac{1}{5}} Z^{\frac{2}{5}}$.*

(ii) If $B \le Z$ expression (26.3.24) *does not exceed $C(B+1)^{\delta} Z^{\frac{2}{3}-\delta}$.*

Trace Term

Let us consider the *trace term* i.e. expression $\int e_1(x,x,\nu)\,dx = \operatorname{Tr}((H-\nu)^-)$.

Regular Zone. Here again let us consider first zone where $|x| \le (1-\epsilon)\bar{r}$. Then the contribution of $B(x,\ell(x))$ to the Tauberian remainder[21] does not exceed $C\zeta^2(h^{-1}+\mu) \asymp C\zeta^3\ell + CB\zeta\ell$ as in the mock proof and the summation over zone results in $CZ^{\frac{5}{3}} + CZ^{\frac{4}{3}} B^{\frac{1}{3}} + CZ^{\frac{3}{5}} B^{\frac{4}{5}}$.

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[21] We will consider a bit later transition from the Tauberian expression to the magnetic Weyl expression.

Border Strip. Again in zone $\mathcal{Y}_1$ contribution of $B(x,\gamma(x))$ does not exceed $CB\varsigma\ell_1$ and the summation over this zone returns

$$CB\int \varsigma\ell_1^{-2}\,dx \tag{26.3.73}$$

and plugging $\ell_1=\bar{r}\gamma$ and $\varsigma=\bar{\zeta}\gamma^2$ results in $CB^{\frac{5}{4}}$ as $B\lesssim Z^{\frac{4}{3}}$ and $CB^{\frac{4}{5}}Z^{\frac{3}{5}}$ otherwise. The analysis of zone $\mathcal{Y}_0$ if there $\mathcal{Y}_2=\emptyset$ is also easy.

Consider zones $\mathcal{Y}_2$ and $\mathcal{Y}_0$. The same arguments as before imply that their contributions to the remainder do not exceed $CB\bar{r}^2\bar{\varsigma}\bar{\ell}_1^{-1}$ which is what we got before.

Justification: from Tauberian to Magnetic Weyl Expression.

Case $\mu h\le C_0$. We need to prove that with the announced error we can replace the Tauberian expression by magnetic Weyl one. Note that the canonical form of $\zeta^{-2}H_{A,W}$ as described in Sections 13.3 and 18.7 is

$$\begin{aligned}\mathcal{H}=\mathcal{H}_0+&\\ &\mu^{-2}\omega_1(x_1,\mu^{-1}hD_1,x_3)+\mu^{-2}\omega_2(x_1,\mu^{-1}hD_1,x_3)(x_2^2+\mu^2h^2D_2^2)\\ &\qquad+\mu^{-1}h\omega_3(x_1,\mu^{-1}hD_1,x_3)+O\bigl(\mu^{-3}h(\gamma+\mu^{-1})^{-\frac{3}{2}}+\mu^{-4}\bigr)\end{aligned} \tag{26.3.74}$$

with

$$\mathcal{H}_0=h^2D_3^2-(x_2^2+\mu^2h^2D_2^2\pm\mu h)+w(x_1,\mu^{-1}hD_1,x_3) \tag{26.3.75}$$

and

$$\gamma=\epsilon\min_j|w-2j\mu h| \tag{26.3.76}$$

where we used the fact that $w\in\mu h\mathscr{C}^{\frac{5}{2}}+\mathscr{C}^n$, $\mu^{-3}h=\mu^{-4}\cdot\mu h$. Here we have signs "+" and "−" on $q/2$ of the diagonal elements equally.

Then the Tauberian expression is

$$\begin{aligned}\mathsf{const}\cdot\mu h^{-2}\int\sum_{j\ge0}\bigl(w-2j\mu h-\mu^{-2}\omega_1-2j\mu^{-1}h\omega_2\bigr)_+^{\frac{3}{2}}\times&\\ \bigl(\psi+\mu^{-2}\psi_1+2j\mu^{-1}h\psi_2\bigr)\,dx&\end{aligned} \tag{26.3.77}$$

where term with $j=0$ enters with the weight $\frac{1}{2}$ and an error does not exceed

$$Ch^{-3}\Bigl(\mu^{-4}+\mu^{-3}h\int (\gamma+\mu^{-1})^{-\frac{3}{2}}\,dx\Bigr)\asymp C\mu^{-\frac{7}{2}}h^{-3}$$

because an integral does not exceed $C\mu^{\frac{1}{2}}(\mu h)^{-1}$; since $\mu\ge h^{-\frac{3}{5}}$ this error does not exceed $Ch^{-\frac{9}{10}}$ which is better than $O(h^{-1})$.

On the other hand, if we consider the difference between (26.3.77) and the same expression with $\omega_1=\omega_2=\psi_1=\psi_2=0$ and consider it as a Riemannian sum and replace it by an integral we get $G\mu^{-2}h^{-3}$ with an error not exceeding $C\mu^{-4}(\mu h)^{\frac{1}{2}}h^{-3}$ which is even less. Therefore (26.3.77) becomes

$$\int P_{\mu h}(w)\psi\,dx+G\mu^{-2}h^{-3}$$

and comparing with the result if $\mu\asymp h^{-\frac{3}{5}}$ when we get the same answer albeit with $G=0$ we conclude that G *must* be 0. This concludes the justification in $\mathcal{X}_2$.

Case $\mu h\ge C_0$. In this case we need a simplified version of (26.3.74) $\mathcal{H}=\mathcal{H}_0+O(\mu^{-1}h)$ and we need to consider only $j=0$ and replacing $\mathcal{H}$ by $\mathcal{H}_0$ brings and error $C\mu h^{-2}\times\mu^{-1}h=O(h^{-1})$. This takes care of $\mathcal{X}_2$ and after scaling of $\mathcal{Y}$.

Conclusion. As $Z^2\le B\le Z^3$ we need to estimate also contribution of $\mathcal{X}_0=\{x\colon \ell(x)\le CZ^{-1}\}$. By means of variational methods we will prove (see Corollary 26.A.5)

(26.3.78) For $Z^2\le B\le Z^3$ the contributions of $\mathcal{X}_0$ to both $\int e_1(x,x,\nu)\,dx$ and $\int P'_B(W(x)+\nu)\,dx$ do not exceed CB.

Then we arrive to the following

Proposition 26.3.17. *Let $M=1$. Then*

(i) For constructed above potential W expression (26.3.26) *does not exceed $CZ^{\frac{5}{3}}+CZ^{\frac{4}{3}}B^{\frac{1}{3}}+CZ^{\frac{3}{5}}B^{\frac{4}{5}}$.*

(ii) If $B\le Z$ expression (26.3.26) *does not exceed $C(B+1)^{\delta}Z^{\frac{5}{3}-\delta}$ (but one should subtract a Schwinger term from the trace).*

Semiclassical D-Term: Local Theory

Unfortunately, we do not have any non-smooth theory (cf. Section 16.8) here so far but actually we almost do not need it since singularities are rather rare. Let us introduce a scaling function (26.3.76) and consider

$$J_\lambda(z) = \int \phi_{z,\lambda}(x)\bigl(e(x,x,\tau) - P_\beta(w(x)+\tau)\bigr)\,dx \tag{26.3.79}$$

with $\phi_{z,\lambda}(x) = \phi(\lambda^{-1}(x-z))$ and $\lambda \le \gamma(z)$. Scaling $x \mapsto \lambda^{-1}(x-z)$ we have $\mu \mapsto \mu' = \lambda\mu$ and $h \mapsto h' = \lambda^{-1}h$.

Then, according to Section 13.5

$$|J_\lambda(z)| \le Ch'^{-2}(1+\mu' h') \asymp C\lambda^2 h^{-2}(1+\mu h) \tag{26.3.80}$$

as long as $\lambda \ge h$.

Really, a transition from the Tauberian decomposition to magnetic Weyl one in this case is easy: skipping all perturbation terms $O(\mu^{-2}+\mu^{-1}h)$ in (26.3.74) and also setting $\psi_1=\psi_2=0$ results in an error $O\bigl(\mu^{-2}h^{-3}+h^{-1}\bigr)$ in (26.3.77)-like expression albeit with the power $\frac{1}{2}$ rather than $\frac{3}{2}$ and without integration:

$$\mathsf{const}\cdot \mu h^{-2}\sum_{j\ge 0}\bigl(w - 2j\mu h - \mu^{-2}\omega_1 - 2j\mu^{-1}h\omega_2\bigr)_+^{\frac{1}{2}}\times \\ \bigl(\psi + \mu^{-2}\psi_1 + 2j\mu^{-1}h\psi_2\bigr); \tag{26.3.81}$$

scaling produces expression smaller than (26.3.80).

Let us apply this estimate (26.3.80) to the Fefferman–de Llave decomposition (26.3.8).

Case $\mu \le C_0 h^{-1}$.

(i) Consider first a pair (z,z') such that $|z'-z''| \le \epsilon_0\gamma(z')$; then also $|z'-z''| \le \epsilon_0\gamma(z'')$ and we take $\lambda = \epsilon|z'-z''|$.

Then in the virtue of (26.3.80) the total contribution to D-term of all such pairs belonging to $B(z,\gamma(z))$, and with $|z'-z''|\asymp\lambda$ does not exceed

$$C\gamma^3\lambda^{-3}\times\lambda^{-1}\times\lambda^2h^{-4}(1+\mu h)^2 \asymp C\gamma^3h^{-4}(1+\mu h)^2 \tag{26.3.82}$$

where $C\gamma^3\lambda^{-3}$ estimate the number of such pairs, λ^{-1} the inverse distance between them, and $C\lambda^2h^{-2}(1+\mu h)$ is the right-hand expression of (26.3.80).

Then summation over $\lambda\in(\mu^{-1},\gamma)$ results in $C\gamma^3(1+\mu h)^2h^{-4}|\log(\mu\gamma)|$.

Further, summation over all balls $B(z,\gamma)\subset B(0,1)$ with $\gamma(z)\asymp\gamma$ results in $C(\mu h)^{-1}\gamma h^{-4}|\log(\mu\gamma)|$ since there are $\asymp(\mu h)^{-1}\gamma^{-2}$ such balls due to non-degeneracy assumption $|\nabla w|\asymp 1$. Summation over $\gamma\in(\mu^{-1},\mu h)$ results in $Ch^{-4}|\log(\mu^2h)|$.

As $\lambda\le\mu^{-1}$ we can apply standard non-magnetic methods without Fefferman–de Llave decomposition (26.3.8). Coefficients are smooth after scaling as long as $\varepsilon\ge\mu^{-1}$.

(ii) Consider *disjoint* pairs (z',z'') with $|z'-z''|\ge\max\bigl(\gamma(z'),\gamma(z'')\bigr)$. Here estimate (26.3.80) is not sufficient and it should be replaced by

$$|J_\gamma(z)|\le C\lambda^3h^{-2}(1+\mu h) \tag{26.3.83}$$

as long as

$$\gamma\ge h^{\frac{2}{3}-\delta}. \tag{26.3.84}$$

Really, the shift for time T with respect to ξ_3 is $\asymp T$ provided $|\nabla_{x_3}w|\asymp 1$ and this shift is observable if $T\times\gamma\gtrsim h^{1-\delta}$. Similarly, in the canonical form the shift for time T with respect to $\mu^{-1}\xi_i$ is $\asymp\mu^{-1}T$ provided $|\nabla_{x_i}w|\asymp 1$ and this shift is observable if $\mu^{-1}T\times\gamma\gtrsim\mu^{-1}h^{1-\delta}$. In both cases shift with $T\in(\gamma^{\frac{1}{2}},\epsilon_0)$ is observable under assumption (26.3.84) and therefore we can extend $T\asymp\gamma^{\frac{1}{2}}$ to $T\asymp 1$.

Note that for $\varepsilon\ge h^{\frac{2}{3}-\delta}$ assumption (26.3.84) is fulfilled automatically. Then contribution of each disjoint pair to D-term does not exceed

$$Ch^{-4}(1+\mu h)^2\gamma(z')^3\gamma(z'')^3|z'-z''|^{-1}$$

and the total contribution does not exceed

$$Ch^{-4}(1+\mu h)^2\iint |z'-z''|^{-1}\,dz'dz''\asymp Ch^{-4}(1+\mu h)^2.$$

(iii) To shed of logarithm in (i) we need a slightly better estimate than (26.3.80). The same arguments as in Part (ii) result in

$$|J_\lambda(z)|\le C\lambda^2h^{-2}(1+\mu h)\cdot(1+\lambda\gamma/h)^{-\delta}. \tag{26.3.85}$$

Really, we just advance from time $T\asymp\lambda$ to $T\asymp\lambda(1+\lambda\gamma/h)^{\delta}$.

Then the same factor is acquired by the right-hand expression of (26.3.82) and the summation with respect to $\lambda \in (h\gamma^{-1}, \gamma)$ results in $C\gamma^3(1+\mu h)^2 h^{-4}$ but summation with respect to $\lambda \in (\mu^{-1}, h\gamma^{-1})$ results

$$C\gamma^3(1+\mu h)^2 h^{-4}\bigl(1+|\log(\mu h\gamma^{-1})|\bigr).$$

Further, summation over all balls $B(z,\gamma)\subset B(0,1)$ with $\gamma(z)\asymp\gamma$ results in $C(\mu h)^{-1}\gamma(1+\mu h)^2 h^{-4}\bigl(1+|\log(\mu h\gamma^{-1})|\bigr)$ and, finally, summation over $\gamma\lesssim \mu h$ results in $Ch^{-4}(1+\mu h)^2$.

Note that in all cases perturbation terms in (26.3.74) and (26.3.81) result in the error not exceeding the announced one.

Case $\mu \ge C_0 h^{-1}$. So far factor $(1+\mu h)$ was for a compatibility only. Now it is important.

Exactly the same arguments work as $\mu \ge C_0 h^{-1}$ with a minor modifications:

(a) $\gamma(x)$ now is defined by (26.3.76) with $j=0$ and its upper bound is 1 rather than μh.

(b) Also the number of γ-balls is $\asymp \gamma^{-2}$ rather than $\asymp (\mu h)^{-1}\gamma^{-2}$;

(c) λ now runs from h to γ in (i) and (iii).

(d) We need to estimate contribution of pairs (z',z'') with $|z'-z''|\le h$. One can see easily that $e(x,x,\tau)\le \mu h^{-2}$ and therefore the total contribution of these pairs does not exceed $C\mu^2 h^{-4}\iint |z'-z''|^{-1}\,dz'dz'' \asymp C\mu^2 h^{-4}\times h^2 \asymp C\mu^2 h^{-2}$.

Therefore we have the following

Proposition 26.3.18. *As $|\nabla w|\asymp 1$ and $\varepsilon \ge h^{\frac{2}{3}-\delta}$ in $B(0,1)$ and $\phi\in \mathscr{C}^\infty(B(0,\frac{1}{2})$*

$$\mathsf{D}\Bigl(\phi\bigl(e(x,x,\tau)-P'_\beta(w(x)+\tau)\bigr),\phi\bigl(e(x,x,\nu)-P'_\beta(w(x)+\tau)\bigr)\Bigr)\le C(1+\mu h)^2 h^{-4}. \tag{26.3.86}$$

Remark 26.3.19. One can see easily that one can select $\varepsilon \ge h^{\frac{2}{3}-\delta}$ such that expressions (26.3.61), (26.3.62) and (26.3.62) will be respectively $O(h^{2+\delta})$, $O(h^{1+\delta})$ and $O(h^{2+\delta})$.

Semiclassical D-Term: Global Theory

Regular Zone. The above results allow us to consider a total contribution of zone $\mathcal{X}_2$ into semiclassical D-term. As before let us consider ℓ-admissible partition of unity there and apply it to Fefferman–de Llave decomposition (26.3.8). Then the total contribution of the elements which are not disjoint does not exceed

$$\sum_n \ell_n^{-1}\bigl(1 + B\zeta_n^{-2}\bigr)^2 \ell_n^4\zeta_n^4 \asymp \int \underbrace{(\zeta^4 + B^2)\ell^3}\, \ell^{-1}d\ell \tag{26.3.87}$$

where $\bigl(1 + B\zeta_n^{-2}\bigr)^2$ and $\ell_n^4\zeta_n^4$ are $(1+\mu h)$ and h^{-4} respectively and ℓ_n^{-1} is a scaling factor.

Then if $\zeta^2 = Z\ell^{-1}$, an integral equals to the value of the selected expression as ℓ reaches its maximum, i.e. for $\ell = Z^{-\frac{1}{3}}$ for $B \le Z^{\frac{4}{3}}$ and $\ell = Z^{\frac{1}{5}}B^{-\frac{2}{5}}$ for $Z^{\frac{4}{3}} \le B \le Z^3$ and we arrive to $CZ^{\frac{5}{3}}$ and $CZ^{\frac{3}{5}}B^{\frac{4}{5}}$ respectively.

On the other hand, if $\zeta^2 = \ell^{-4}$ an integral equals to the value of the selected expression as ℓ reaches its minimum, i.e. for $\ell = Z^{-\frac{1}{3}}$ and only in the case $B \le Z^{\frac{4}{3}}$ and we arrive to $CZ^{\frac{5}{3}}$ again.

Furthermore, the total contribution of the disjoint elements does not exceed

$$\sum_{n,p} |z_n - z_p|^{-1}\bigl(1 + B\zeta_n^{-2}\bigr)\bigl(1 + B\zeta_p^{-2}\bigr)\ell_n^2\zeta_n^2\ell_p^2\zeta_p^2 \asymp \iint \underbrace{(\ell+\ell')^{-1}(\zeta^2 + B)\ell^2(\zeta'^2 + B)\ell'^2}\, \ell^{-1}d\ell\,\ell'^{-1}d\ell'. \tag{26.3.88}$$

Then if $\zeta^2 = Z\ell^{-1}$ and $\zeta'^2 = Z\ell'^{-1}$ an integral equals to the value of the selected expression as both ℓ and ℓ' reach their maxima, and we arrive to $CZ^{\frac{5}{3}}$ and $CZ^{\frac{3}{5}}B^{\frac{4}{5}}$ respectively.

On the other hand, if $\zeta^2 = \ell^{-4}$ and $\zeta'^2 = \ell'^{-4}$ (we do not need to consider mixed pair) an integral equals to the value of the selected expression as both ℓ and ℓ' reach their minima, and we arrive to $CZ^{\frac{5}{3}}$.

Therefore (combining with Proposition 26.A.5 as $Z^2 \le B \le Z^3$) we arrive to

Proposition 26.3.20. *Let $M = 1$. Then* *(i) The total contribution of the zone* $\{x\colon \ell(x)\le (1-\epsilon)\bar{r}\}$ *to the semiclassical* D*-term does not exceed* $CZ^{\frac{5}{3}}$ *and* $CZ^{\frac{3}{5}}B^{\frac{4}{5}}$ *for* $B\le Z^{\frac{4}{3}}$ *and for* $Z^{\frac{4}{3}}\le B\le Z^3$ *respectively.*

(ii) If $B\le Z$ *this contribution does not exceed* $C(B+1)^{\delta}Z^{\frac{5}{3}-\delta}$*.*

Border Strip. Border strip $\mathcal{Y}=\{x\colon (1-\epsilon)\bar{r}\le \ell(x)\le (1+\epsilon)\bar{r}\}$ is more subtle. Here we need to use the same $\ell_1(x)=\epsilon_0(\bar{r}-|x|)$ partition as before.

Remark 26.3.21. $\mathcal{Y}$ is already covered by our arguments if $\bar{r}\asymp (Z-N)_+^{-\frac{1}{3}}$.

Close Elements. Consider first contribution of elements which are not disjoint. It is given by the left-hand expression of (26.3.87) with ℓ, ζ replaced by $\ell_1(x)=\bar{r}\gamma(x)$ and $\varsigma(x)=\bar{\zeta}\gamma(x)^2$ respectively. However since the layer $\{x\colon \gamma(x)\asymp\gamma\}$ contains $\asymp\gamma^{-2}$ elements the right-hand expression should be replaced by

$$\int \underbracket{B^2\bar{r}^3\gamma}\,\gamma^{-1}d\gamma\asymp B^2\bar{r}^3$$

since $\varsigma^2\le B$; so we arrive to $O\bigl(\max(B^{\frac{5}{4}}, Z^{\frac{3}{5}}B^{\frac{4}{5}}\bigr)$.

Meanwhile for $\mathcal{Y}_2$ we have $\gamma(x)=\bar{\gamma}\le 1$ and $\varsigma(x)=\bar{\varsigma}=\bar{\zeta}\bar{\gamma}^2$ and its contribution does not exceed what we got for $\mathcal{Y}_1$.

Disjoint Elements. Consider contribution of the disjoint elements. It is given by the left-hand expression of (26.3.88) with ℓ, ζ replaced by γ and ς respectively. Note that $\sum_{n,p}|z_n-z_p|^{-1}\asymp \bar{r}^{-1}\gamma^{-2}\gamma'^{-2}$ where we sum with respect to all pairs with $\gamma_n\asymp\gamma$ and $\gamma_p\asymp\gamma'$. Therefore the right-hand expression should be replaced by

$$\int \underbracket{\bar{r}^3B^2}\,\gamma^{-1}d\gamma\,\gamma'^{-1}d\gamma' \tag{26.3.89}$$

which leads to $C\bar{r}^3B^2|\log(\bar{r}^{-1}\bar{\gamma})|^2$ which differs from what we got before by a logarithmic factor. To get rid of it we will use exactly the same trick as in Paragraph *26.3.3.2.2. Border Strip* proving Proposition 26.3.16 because considering disjoint pairs we consider the same objects as there. Then instead of (26.3.89) we arrive to

$$\int \underbracket{\bar{r}^3B^2\gamma^{-\delta}\gamma'^{-\delta}\bar{\gamma}^{2\delta}}\,\gamma^{-1}d\gamma\,\gamma'^{-1}d\gamma'$$

which results in $C\bar{r}^3 B^2$.

Meanwhile for $\mathcal{Y}_2$ we have $\gamma(x) = \bar{\gamma} \leq \bar{r}$ and $\varsigma(x) = \bar{\varsigma} = \bar{\zeta}\bar{\gamma}^2$ and its contribution does not exceed what we got for $\mathcal{Y}_1$.

Conclusion. Finally, analysis in the outer zone is trivial. Therefore we arrive

Proposition 26.3.22. *Let $M = 1$. Then for constructed above potential W*

(i) Expression (26.3.25) *does not exceed $CZ^{\frac{5}{3}} + CZ^{\frac{3}{5}}B^{\frac{4}{5}}$.*

(ii) If $B \leq Z$ expression (26.3.25) *does not exceed $C(B+1)^{\delta}Z^{\frac{5}{3}-\delta}$.*

26.4 Applying Semiclassical Methods: $M \geq 2$

Let us consider now the molecular case ($M \geq 2$). The major problem is that the non-degeneracy condition $|\nabla w| \asymp 1$ is not necessarily fulfilled. Therefore we need to find an alternative approach to the zone where $\mu \geq h^{-\frac{1}{3}}$) (with $\mu = B\ell\zeta^{-1}$ and $h = 1/\ell\zeta$). Recall that it consists of three smaller zones: zone $\mathcal{X}_2 := \{\mu h \leq C_0,\ W_B^{\mathsf{TF}} \geq \epsilon_0\zeta^2\}$ [22], zone $\mathcal{X}_3 := \{\mu h \geq C_0,\ W_B^{\mathsf{TF}} \geq \epsilon_0\zeta^2\}$ [23], and the (most difficult) *boundary strip* $\mathcal{Y} = \{W_B^{\mathsf{TF}} \leq \epsilon_0\zeta^2\}$, which we leave for the next Section 26.5.

26.4.1 Scaling Functions in Zone $\mathcal{X}_2$

Step 1. We will use the scaling method in this zone; the good news is that W_B^{TF} is sufficiently regular after a proper rescaling and also sufficiently non-degenerate. Recall that after we rescale $x \mapsto \bar{\ell}^{-1}(x-\bar{x})$, $\tau \mapsto \bar{\zeta}^{-2}\tau$ in the ball $B(\bar{x}, \frac{1}{2}\bar{\ell})$ with $\bar{\ell} = \ell(\bar{x})$, $\bar{\zeta} = Z^{\frac{1}{2}}\bar{\ell}^{-1}$, the rescaled potential $w = \bar{\zeta}^{-2}W_B^{\mathsf{TF}}$ satisfies in $B(0,2)$ equation

$$\frac{1}{4\pi}\Delta w = \eta P'_{\beta}(w) \qquad \text{with } \ \eta = \bar{\zeta}\bar{\ell}^2 \lesssim 1, \quad \beta = \mu h = B\bar{\zeta}^{-2} \leq 1 \tag{26.4.1}$$

and therefore in $B(0,1)$

$$w = -\frac{1}{4\pi}\int |x-z|^{-1}\eta P'_{\beta}(w(z))\phi(z)\,dz + w' \tag{26.4.2}$$

[22] Only if $B \leq C_1 Z^2$; this zone disappears for $C_1 Z^2 \leq B \lesssim Z^3$.
[23] Only if $Z^{\frac{4}{3}} \lesssim B \lesssim Z^3$; this zone disappears for $B \lesssim Z^{\frac{4}{3}}$.

with $\phi \in \mathscr{C}_0^\infty(B(0,\frac{5}{6}))$ and $w' \in \mathscr{C}_0^\infty(B(0,\frac{3}{4}))$.

Remark 26.4.1. (i) If $\zeta^2 \asymp Z\ell^{-1}$ then $\eta = Z^{\frac{1}{2}}\ell^{\frac{3}{2}} \le 1$; this happens for $B \le Z^{\frac{4}{3}}$, $\ell \lesssim Z^{-\frac{1}{3}}$ and for $B \ge Z^{\frac{4}{3}}$, $\ell \lesssim B^{-\frac{1}{3}}$.

(ii) If $\zeta^2 \asymp \ell^{-2}$ then $\eta \asymp 1$; this happens only for $B \le Z^{\frac{4}{3}}$, $\ell \gtrsim Z^{-\frac{1}{3}}$.

Let us introduce a function

$$\gamma_0(x) = \Bigl(\min_j |w - 2j\beta|^3 + |\nabla w|^4 + |\nabla^2 w|^6 + |\nabla^3 w'|^{12}\Bigr)^{\frac{1}{12}}. \tag{26.4.3}$$

Remark 26.4.2. We cannot replace w' by w in the last term because $w \in \mathscr{C}^{\frac{5}{2}}$ only rather than $\mathscr{C}^3$.

Proposition 26.4.3. *$\gamma_0(x)$ is a scaling function i.e. $|x-y| \le \epsilon\gamma_0(x) \implies \gamma_0(y) \asymp \gamma_0(x)$.*

Proof. (a) If w belonged to $\mathscr{C}^4$ (and we would put w instead of w' in the last term of (26.4.3)) then we would just prove that $|\nabla\gamma_0| \le c$. Here we should be more subtle. We need to prove that if

$$\min_j |w - 2j\beta| \le \gamma_0^4, \qquad |\nabla w| \le \gamma_0^3, \tag*{$(26.4.4)_{1,2}$}$$

$$|\nabla^2 w| \le \gamma_0^2, \qquad |\nabla^3 w'| \le \gamma_0 \tag*{$(26.4.4)_{3,4}$}$$

at point x, then at point y the same inequalities hold with γ_0 replaced by $c\gamma_0$ [24]. Definitely this is true for $(26.4.4)_4$ since w' is smooth.

(b) Consider $|\nabla^2 w|$. Consider $|\Lambda_\alpha w(y) - \Lambda_\alpha w(x)|$ with $\Lambda_\alpha = \nabla^\alpha - \frac{1}{3}\delta_{ij}\Delta$, $\alpha = (i,j)$. Then due to (26.4.2)

$$\begin{aligned} &|\Lambda_{\alpha,y} w(y) - \Lambda_{\alpha,x} w(x)| \le \\ &\qquad |\eta \int \bigl(\Lambda_{\alpha,x}|x-z|^{-1} - \Lambda_{\alpha,y}|y-z|^{-1}\bigr) P'_\beta(w(z))\phi(z)\,dz| + \epsilon_1\gamma_0^2 \end{aligned} \tag{26.4.5}$$

where the last term estimates $|\Lambda_{\alpha,y} w'(y) - \Lambda_{\alpha,x} w'(x)|$ and we used $(26.4.4)_4$. Integrals here are understood in the sense of the principal value (vrai) and $\epsilon_1 = \epsilon_1(\epsilon) \to +0$ as $\epsilon \to +0$.

[24] We need to prove a bit of converse as well; see Part (c).

Note that the integral in expression (26.4.5) does not change if we add to $P'_\beta(w)$ any constant with respect to z.

Let us consider first this integral over $\{z\colon |x-z|\geq 2\gamma_0\}$, provided $\gamma_0\geq |x-y|$, and note that this integral does not exceed

$$\eta|\int |x-z|^{-4}|x-y|\times \\ \bigl(|\nabla w(x)|\cdot |x-z| + |\nabla^2 w(x)|\cdot |x-z|^2 + |x-z|^{\frac{5}{2}}\bigr)^{\frac{1}{2}}\, dz| \leq C\epsilon_1\eta.$$

Consider now integral over zone $\{z\colon |x-z|\leq 2\gamma_0\}$:

$$|\eta\int \Lambda_{\alpha,x}|x-z|^{-1}\cdot \bigl(P'_\beta(w(z)) - P'_\beta(w(x))\bigr)\, dz|$$

and note that it also does not exceed $\epsilon_1\eta$. Further, t same arguments work for this integral with x replaced by y but still integrated over zone $\{z\colon |x-z|\leq 2\gamma_0\}$ (one needs to remember that $|\nabla w(x) - \nabla w(y)| = O(\gamma_0)$ and $|\nabla^2 w(x) - \nabla^2 w(y)| = O(\gamma_0^{\frac{1}{2}})$).

Furthermore, the same arguments work also for these expressions integrated over $\{z\colon |y-z|\leq 2\gamma_0\}$ and we are left with

$$|\eta\int \omega(x,y,z)\bigl(P'_\beta(w(x)) - P'_\beta(w(y))\bigr)\, dz|$$

integrated over zone $\{z\colon |x-z|\asymp \gamma_0\}$ and $\omega\asymp\gamma_0^{-3}$ and one can estimate it by $\epsilon_1\eta$ easily in the same way. Therefore since $|\Delta w(x) - \Delta w(y)|$ does not exceed $\epsilon_1\eta$ we conclude that $|\nabla^2 w(x) - \nabla^2 w(y)|$ does not exceed $\epsilon_1(\eta+\gamma_0^2)$.

However (26.4.2) implies that $\eta\leq c\gamma_0^2$ since $P'_\beta(w)\asymp 1$ in $\mathcal{X}_2$ and therefore $|\nabla^2 w(x) - \nabla^2 w(y)|\leq \epsilon_1\gamma_0^2$ in $B(x,\gamma_0)$.

Finally, combining this inequality with $(26.4.4)_2$ we conclude that $|\nabla w(x) - \nabla w(y)|\leq \epsilon_1\gamma_0^3$ in $B(x,\gamma_0)$; finally, combining with $(26.4.4)_1$ we conclude that $|w(x) - w(y)|\leq \epsilon_1\gamma_0^4$ in $B(x,\gamma_0)$.

(c) Therefore $(26.4.4)_{1-4}$ are fulfilled in $y\in B(x,\epsilon\gamma_0)$ with γ_0 replaced by $\gamma_0(1+C\epsilon_1)$. Further, if we redefine γ_0 as the minimal scale such that inequalities $(26.4.4)_{1-4}$ are fulfilled in x, then $(26.4.4)_{1-4}$ fail in $y\in B(x,\epsilon\gamma_0)$ with γ_0 replaced by $\gamma_0(1-C\epsilon_1)$. Therefore with appropriate $\epsilon>0$ we conclude that $\frac{1}{2}\leq \gamma_0(x)/\gamma_0(y)\leq 2$.

Obviously, $\gamma_0 \asymp \gamma_{0\mathsf{old}}$ where $\gamma_{0\mathsf{old}}$ was defined by (26.4.3) and therefore the same conclusion also holds for $\gamma_{0\mathsf{old}}$. $\square$

Now let us reintroduce the scaling function

$$\gamma_0(x) = \epsilon\Bigl(\min_j |w - 2j\beta|^3 + |\nabla w|^4 + |\nabla^2 w|^6 + |\nabla^3 w'|^{12}\Bigr)^{\frac{1}{12}} + C_0 h^{\frac{1}{3}} + C_0\eta^{\frac{1}{2}}. \tag{26.4.3*}$$

Then

(26.4.6) $|x-y| \le 2\gamma_0(x) \implies \gamma_0(y) \asymp \gamma_0(x)$ and $(26.4.4)_{1-4}$ hold (with some constant factor in the right-hand expression).

Consider $B(\bar{x},\bar{\gamma}_0)$, $\bar{\gamma}_0 = \gamma_0(\bar{x})$, and scale again $x \mapsto \bar{\gamma}_0^{-1}(x-\bar{x})$, $\tau \mapsto \bar{\gamma}_0^{-4}\tau$ and respectively $w \mapsto w_1 = \bar{\gamma}_0^{-4}(w - 2\bar{j}\beta))$, $h \mapsto h_1 = h\bar{\gamma}_0^{-3}$. Further, since after rescaling $|\Delta w_1| = O(\eta\bar{\gamma}_0^{-2})$ we set $\eta \mapsto \eta_1 = \eta\bar{\gamma}_0^{-2}$.

Due to cut-off in the end of (26.4.3)* $h_1 \lesssim 1$ and $\eta_1 \lesssim 1$. If $\bar{\gamma}_0 \asymp h^{\frac{1}{3}}$ then $h_1 \asymp 1$ and we are done. If $\bar{\gamma}_0 \asymp \eta^{\frac{1}{2}}$ then $\eta_1 \asymp 1$ and we proceed to *Step 3*.

Step 2. So, let $\eta_1 \ll 1$. Let us introduce a scaling function in $B(0,1)$ obtained after the previous rescaling:

$$\gamma_1(x) = \epsilon\Bigl(\min_j |w_1 + 2(\bar{j}-j)\beta\bar{\gamma}_0^{-4}|^2 + |\nabla w_1|^3 + |\nabla^2 w_1|^6\Bigr)^{\frac{1}{6}}. \tag{26.4.7}$$

Then

$$\min_j |w_1 + 2(\bar{j}-j)\beta\bar{\gamma}_0^{-4}| \le C_0\gamma_1^3, \qquad |\nabla w_1| \le C_0\gamma_1^2, \tag{26.4.8$_{1-2}$}$$

$$|\nabla^2 w_1| \le C_0\gamma_1. \tag{26.4.8$_3$}$$

Remark 26.4.4[25]. Since now we do not have the third derivative in (26.4.7), we do not need in w'_1 in the definition of γ_1, only in the proof of Proposition 26.4.5 below.

Proposition 26.4.5. *(i)* $\gamma_1(x)$ *is a scaling function:* $|x-y| \le 2\gamma_1(x) \implies \gamma_1(y) \asymp \gamma_1(x)$.

[25] Cf. Remark 26.4.2.

(ii) If $\eta_1 \le \epsilon_0$ *then*

$$|\nabla^2 w_1(x) - \nabla^2 w_1'(x)| \le \epsilon_2\gamma_1, \qquad w_1' = (w' - \bar{\jmath}\beta)\gamma_0^{-4}. \tag{26.4.9}$$

Proof. Proof is similar but simpler than one of Proposition 26.4.3; it is based on the rescaled version of (26.4.1)–(26.4.2):

$$\frac{1}{4\pi}\Delta w_1 = \eta_1 P_\beta(w_1\bar{\gamma}_0^4 + 2\bar{\jmath}\beta), \qquad \eta_1 = \eta\bar{\gamma}_0^{-2} \le 1 \tag{26.4.10}$$

and therefore in $B(0,1)$

$$w_1 = -\frac{1}{4\pi}\int |x-z|^{-1}\eta_1 P_\beta'(w_1(z)\bar{\gamma}_0^4 + 2\bar{\jmath}\beta)\phi(z)\,dz + w_1'. \tag{26.4.11}$$

$\square$

Now let us reintroduce the scaling function

$$\gamma_1(x) = \epsilon\Bigl(\min_j |w_1 + 2(\bar{\jmath} - j)\beta\bar{\gamma}_0^{-4}|^2 + |\nabla w_1|^3 + |\nabla^2 w_1|^6\Bigr)^{\frac{1}{6}} + C_0 h_1^{\frac{2}{5}}. \tag{26.4.7*}$$

Then

(26.4.12) $|x-y| \le 2\gamma_0(x) \implies \gamma_0(y) \asymp \gamma_0(x)$ and $(26.4.8)_{1-3}$ hold (with some constant factor in the right-hand expression).

Let us consider $\bar{x} \in B(0,1)$ (it is a new point), $B(\bar{x},\bar{\gamma}_1)$, $\bar{\gamma}_1 = \gamma_1(\bar{x})$, and scale again $x \mapsto \bar{\gamma}_1^{-1}(x-\bar{x})$, $\tau \mapsto \bar{\gamma}_1^{-3}\tau$ and respectively $w_1 \mapsto w_2 = \bar{\gamma}_1^{-3} w_1$, $h_1 \mapsto h_2 = h_1\bar{\gamma}_1^{-\frac{5}{2}}$.

If $\bar{\gamma}_1 \asymp h_1^{\frac{2}{5}}$ then $h_2 \asymp 1$ and we are done. If $|\nabla w_2| \asymp 1$ we are done as well.

Step 3. So, consider the remaining case $|\nabla^2 w_2| \asymp 1$. Then we introduce the scaling function (now, we have no doubt that this is a scaling function):

$$\gamma_2(x) = \epsilon\Bigl(\min_j |w_2 + 2(\bar{j} - j)\beta\bar{\gamma}_0^{-4}\bar{\gamma}_1^{-3}| + |\nabla w_2|^2\Bigr)^{\frac{1}{2}} + C_0 h_2^{\frac{1}{2}}. \tag{26.4.13}$$

Let us consider $\bar{x} \in B(0,1)$ (it is a new point), $B(\bar{x},\bar{\gamma}_2)$, $\bar{\gamma}_2 = \gamma_2(\bar{x})$, and scale again $x \mapsto \bar{\gamma}_2^{-1}(x-\bar{x})$, $\tau \mapsto \bar{\gamma}_2^{-2}\tau$ and respectively $w_2 \mapsto w_3 = \bar{\gamma}_2^{-2} w_2$, $h_2 \mapsto h_3 = h_2\bar{\gamma}_2^{-2}$.

If $\bar{\gamma}_2 \asymp h_1^{\frac{1}{2}}$ then $h_3 \asymp 1$ and we are done. If $|\nabla w_3| \asymp 1$ we are done as well.

Step 4. Finally, introduce

$$\gamma_3(x) = \epsilon \min_j |w_3 + 2(\bar{j} - j)\beta\bar{\gamma}_0^{-4}\bar{\gamma}_1^{-3}\bar{\gamma}_2^{-2}| + Ch_3^{\frac{2}{3}}. \tag{26.4.14}$$

26.4.2 Zone $\mathcal{X}_2$: Semiclassical N-Term

Now we apply scaling the arguments using scaling functions γ_{1-3} constructed above.

We revert our steps. While we call γ_{1-3} *relative scaling functions* let us introduce *absolute scaling functions* $\alpha_0(x) = \gamma_0(x)$, $\alpha_1(x) = \gamma_0(x)\gamma_1(x)$, $\alpha_2(x) = \gamma_0(x)\gamma_1(x)\gamma_2(x)$, and $\alpha_3(x) = \gamma_0(x)\gamma_1(x)\gamma_2(x)\gamma_3(x)$ [26].

We need first

Proposition 26.4.6. *Consider $B(0,1)$ and assume that in it*

$$|\nabla w| \asymp \theta, \tag{26.4.15}$$

and

$$|\nabla^2 w| \le c\theta. \tag{26.4.16}$$

Let

$$\gamma(x) := \epsilon \min_j |w - 2\mu h j|\theta^{-1} + \hbar^{\frac{2}{3}} \tag{26.4.17}$$

and

$$\varepsilon \ge \hbar^{\frac{2}{3}-\delta}, \qquad \hbar := h\theta^{-\frac{1}{2}}. \tag{26.4.18}$$

Let $\varphi \in \mathscr{C}_0^\infty([-\epsilon_0, \epsilon_0])$. Then for $\alpha \le \bar{\gamma} := \gamma(\bar{x})$,

$$|\int \phi_\alpha(x)\Bigl(e_\varphi(x,x,\tau) - P'_{\mu h,\varphi}\bigl(w(x)+\tau\bigr)\Bigr)\,dx| \le \\ C\mu h^{-1}\alpha^3 + C\mu h^{-1}\alpha^3\bar{\gamma}^{-1}(\hbar\bar{\gamma}^{-\frac{1}{2}}\alpha^{-1})^s \tag{26.4.19}$$

with

$$e_\varphi(x,y,\tau) := \varphi\bigl(h^2 D_{x_3}^2(\mu h)^{-1}\bigr)\,e(x,y,\tau) \tag{26.4.20}$$

and Weyl expression

$$P'_{\beta,\varphi}(w+\tau) = \mathsf{const}\sum_j \beta(w+\tau-2j\mu h)^{\frac{1}{2}}\varphi(w+\tau-2j\mu h) \tag{26.4.21}$$

---

[26] So far we ignore the very first scaling $x \mapsto (x-\bar{x})\ell^{-1}$. Therefore really absolute scaling functions would be $\alpha_j\ell$.

with the standard constant where for each x only one term is present in this sum. Here we take large $s > 0$ as $\hbar \leq \bar{\gamma}\alpha$ and $s = 0$ otherwise.

Proof. The proof is standard and based on the standard reduction to the canonical form, standard estimates for $U(x, y, t)$ a Schwartz kernel of propagator $e^{i\hbar^{-1}\theta^{-1}tH}$:

$$|F_{t\to\hbar^{-1}\tau} \int \bar{\chi}_T(t)\phi_\alpha(x)U_\varphi(x, x, t)\, dx| \leq C\mu h^{-1}\alpha^3 \tag{26.4.22}$$

for $T \asymp 1$ and

$$|F_{t\to\hbar^{-1}\tau} \int \phi_\alpha(x)\bigl(\bar{\chi}_T(t) - \bar{\chi}_{\bar{T}}(t)\bigr)U_\varphi(x, x, t)\, dx| \leq C\mu h^{-1}\alpha^3(\hbar\bar{\gamma}^{-\frac{1}{2}}\alpha^{-1})^s \tag{26.4.23}$$

with $\bar{T} = \epsilon\gamma^{\frac{1}{2}}$ where U_φ is defined similarly to (26.4.20).

Here obviously we can skip in (26.4.19) all perturbation terms in the argument and in ϕ_α transformed. □

Then plugging into (26.4.19) $\alpha = \gamma$ $(= \bar{\gamma})$, we have factor $(h\gamma^{-\frac{3}{2}})^s$ in the second term.

There are two cases: $\theta \leq \mu h$ and $\theta \geq \mu h$.

In the former case $\theta \leq \mu h$, taking the sum over γ-partition of 1-element we estimate the same expressions with ϕ_1 instead of ϕ_γ by their right-hand expressions integrated over $\gamma^{-3}\, d\gamma$ which returns $C\mu h^{-1}$.

On the other hand, in the latter case $\theta \geq \mu h$, let $\lambda = \mu h\theta^{-1}$. Taking the sum over γ_3-partition of λ-element ϕ_λ by the right-hand expressions which returns $C\mu h_2^{-1}\lambda^2$. In this case summation over λ-partition return $C\theta h^{-2}$.

In both cases we arrive to the following estimate:

$$|\int \phi(x)\Bigl(e_\varphi(x, x, \tau) - P'_{\mu h,\varphi}\bigl(w(x) + \tau\bigr)\Bigr)\, dx| \leq C\theta h^{-2} + C\mu h^{-1}. \tag{26.4.24}$$

Applying this estimate after α_2-scaling we conclude that the left-hand expression with $\phi = \phi_{\alpha_2}$ (in the non-scaled settings) does not exceed $C\theta h^{-2}\alpha_2^2 + C\mu h^{-1}\alpha_2^2$. Here the first term is $O(h^{-2}\alpha_2^3)$ and the summation over 1-element returns $O(h^{-2})$.

Consider the second term $C\mu h^{-1}\alpha_2^2 = C\mu h^{-1}\gamma_0^2\gamma_1^2\gamma_2^2$. Then summation over α_2-partition of α_1-element returns

$$C\mu h^{-1}\gamma_0^2\gamma_1^2 \int \gamma_2^2 \times \gamma_2^{-3}\, dx \asymp C\mu h^{-1}\gamma_0^2\gamma_1^2(1 + |\log \hat{\gamma}_2|)$$

where $\hat{\gamma}_k$ is a minimal value of γ_k over γ_{k-1}-element. However in fact there will be no logarithmic factor because in virtue of equation (26.4.1) there is a positive eigenvalue of $\mathsf{Hess}\, w_2$ of the maximal size (cf. Section 5.2.1). Therefore, in fact, we have $C\mu h^{-1}\gamma_0^2\gamma_1^2$.

Now summation over α_1-partition of α_0-element returns

$$C\mu h^{-1}\gamma_0^2 \int \gamma_1^2 \times \gamma_1^{-3}\, dx \asymp C\mu h^{-1}\gamma_0^2(1 + |\log \hat{\gamma}_1|).$$

Finally, summation over α_0-partition of 1-element returns

$$C\mu h^{-1} \int \gamma_0^2(1 + |\log \hat{\gamma}_1|) \times \gamma_0^{-3}\, dx \asymp C\mu h^{-1}\hat{\gamma}_0^{-1}(1 + |\log \check{\gamma}_1|),$$

where $\check{\gamma}_k$ is an absolute minimum of γ_k. However $\gamma_0^2 \ge \eta$ and $\gamma_1 \ge \eta$ and therefore expression above does not exceed $C\mu h^{-1}\eta^{-\frac{1}{2}}(1 + |\log \eta|)$.

Remark 26.4.7. Recall that we estimated only the cut-off expression. To calculate the full expression we need to calculate also the contribution of the zone $\{\xi_3^3 \ge \mu h\}$. However this is easy.

Really, instead of $\varphi(h^2D_3^2/(\mu h))$ consider $\varphi'(h^2D_3^2/\theta)$ with $\varphi' \in \mathscr{C}^\infty([1,4])$ and $\epsilon\mu h \le \theta \le 1$. Without any scaling one can prove easily that such modified expression (26.4.24) does not exceed $C\theta h^{-2}$. We leave easy details to the reader.

Therefore plugging $\theta = 2^n\mu h$ and taking a sum over $n = 0, \dots, \lfloor |\log_2 \mu h| \rfloor$ we get the required expressions. Also note that in such expressions we need to consider perturbed argument $w + \mu^{-2}\omega_1 + j\mu^{-1}h\omega_2$ (all other terms which are $O(\mu^{-4} + \mu^{-\frac{3}{2}}h)$ could be skipped and also a perturbed function transformed).

Remark 26.4.8. (i) However we need to get rid of these perturbations for $\theta \le \mu h^{1-\delta}$ only. Indeed, for $\theta \ge \mu h^{1-\delta}$ we need canonical form *only* to study propagation and calculations could be performed without it. But then getting rid of the perturbation is trivial provided this perturbation does not exceed $C\mu h^{1+\delta}$ which is the case if

$$\mu \geq h^{-\frac{1}{3}-\delta}. \tag{26.4.25}$$

(ii) Note that in the smooth approximation contributions of $\mathcal{X}_1$ is always less than $CZ^{\frac{2}{3}-\delta_1}$, $C\max(Z^{\frac{5}{3}}, Z^{\frac{3}{5}}B^{\frac{4}{5}})Z^{-\delta_1}$ or $C\max(Z^{\frac{5}{3}}, Z^{\frac{3}{5}}B^{\frac{4}{5}})Z^{-\delta_1} + CB^{\frac{1}{2}}Z^{\frac{7}{6}-\delta_1}$ respectively with an exception of the first two and only in the case of the threshold value $\geq Z^{-\frac{1}{3}-\delta_2}$. However in this case $\eta \geq Z^{-\delta_3}$ and the errors of the smooth approximation approach in fact are less than $CZ^{\frac{2}{3}-\delta_4}$, $CZ^{\frac{5}{3}-\delta_4}$ as well. Therefore there are in fact no exception.

(iii) It is important to have $\varepsilon \leq \mu h$ and with $\varepsilon = \hbar^{\frac{2}{3}-\delta}$, $\hbar = h\theta^{-\frac{1}{2}}$ it means $\mu \geq h^{-\frac{1}{3}-\delta}\theta^{\frac{1}{3}-\frac{1}{2}\delta}$ which is due to (26.4.25).

Therefore we conclude that in the completely non-scaled settings with $\phi = \phi_\ell(x)$

$$|\int \phi(x)\Bigl(e(x,x,\tau) - P'_B\bigl(W(x)+\tau\bigr)\Bigr)| \leq \\ C\zeta^2\ell^2 + CB\ell\zeta^{-\frac{1}{2}}(1+|\log \ell^2\zeta|) \tag{26.4.26}$$

where the first term is Ch^{-2} and the second term is $C\mu h^{-1}\eta^{-\frac{1}{2}}(1+|\log\eta|)$; recall that $h^{-1} \asymp \ell\zeta$, $\mu \asymp B\ell\zeta^{-1}$ and $\eta \asymp \ell^2\zeta$. In comparison with the non-degenerate case $|\nabla W_B^{\mathsf{TF}}| \asymp \zeta^2\ell^{-1}$ we acquired the last term.

Assume first that condition (26.2.28) is fulfilled. Then

(i) If $B \leq Z^{\frac{4}{3}}$, $\ell \leq Z^{-\frac{1}{3}}$ we have $\zeta = Z^{\frac{1}{2}}\ell^{-\frac{1}{2}}$ and the right-hand expression of (26.4.26) returns $CZ\ell + CB\ell^{\frac{5}{4}}Z^{-\frac{1}{4}}$ and the summation with respect to ℓ results in its value as $\ell = Z^{-\frac{1}{3}}$ i.e. $CZ^{\frac{2}{3}} + CBZ^{-\frac{2}{3}}$ with the dominating first term.

(ii) If $B \leq Z^{\frac{4}{3}}$, $\ell \geq Z^{-\frac{1}{3}}$ we have $\zeta = \ell^{-2}$ and the right-hand expression of (26.4.26) returns $C\ell^{-2} + CB\ell^2$. We need to sum as long as $\mu h \leq 1$ i.e. $Z^{-\frac{1}{3}} \leq \ell \leq B^{-\frac{1}{4}}$ and the summation returns $CZ^{\frac{2}{3}} + CB^{\frac{1}{2}}$ with the dominating first term.

(iii) If $Z^{\frac{4}{3}} \leq B \leq Z^2$, $\ell \leq B^{-1}Z$ we have $\zeta = Z^{\frac{1}{2}}\ell^{-\frac{1}{2}}$ and the right-hand expression of (26.4.26) returns $CZ\ell + CBZ^{-\frac{1}{4}}\ell^{\frac{5}{4}}$. Then summation results in $CZ^2B^{-1} + CZ^2B^{-\frac{1}{4}}Z \lesssim Z^{\frac{2}{3}}$.

If assumption (26.2.28) is not fulfilled we can estimate in the first term of the right-hand expression of (26.4.26) parameter ζ from above by $\min(Z^{\frac{1}{2}}\ell^{-\frac{1}{2}}, \ell^{-2})$ and in the second term from below by $\zeta_m = \min(Z_m^{\frac{1}{2}}\ell_m^{-\frac{1}{2}}, \ell_m^{-2})$ if $\ell = \ell_m := |x - \mathsf{y}_m|$ and repeat all above arguments.

Therefore we arrive to the Statement (i) of Proposition 26.4.9 below. Furthermore, note that for $B \le Z$ the zone $\mathcal{X}_2$ is contained in the zone $\{x\colon \ell(x) \ge B^{-\frac{3}{10}} \ge Z^{-\frac{3}{10}}\}$ (really, $\mu \ge h^{-\frac{1}{3}}$ in $\mathcal{X}_2$) and we arrive to the Statement (ii) below.

Proposition 26.4.9. *(i) For $B \le Z^2$ the contribution of zone $\mathcal{X}_2$ to the expression*

$$\int \bigl(e(x,x,\nu) - P'_B(W(x)+\nu)\bigr)\,dx \tag{26.4.27}$$

does not exceed $CZ^{\frac{2}{3}}$.

(ii) For $B \le Z$ the contribution of zone $\mathcal{X}_2$ to the expression (26.4.27) *does not exceed $CZ^{\frac{2}{3}-\delta}$.*

26.4.3 Zone $\mathcal{X}_2$: Semiclassical D-Term

Further, we need to estimate the *semiclassical* D*-term*

$$\mathsf{D}\Bigl(\phi_\alpha[e(x,x,\nu) - P'_B(W(x)+\nu)], \phi_\alpha[e(x,x,0) - P'_B(W(x)]\Bigr) \tag{26.4.28}$$

where $\phi_\alpha(x)$ is an α-admissible function. Again we revert our steps.

Consider $B(x,\bar{\alpha}_3)$ and apply Fefferman–de Llave decomposition (26.3.8). Then in the framework of Proposition 26.4.6 contribution of pairs $B(x,\alpha)$ and $B(y,\alpha)$ with $3\alpha \le |x-y| \le 4\alpha$ does not exceed the right-hand expression of (26.4.19) squared and multiplied by α^{-4}, where $C\alpha^{-3}$ estimates the number of the pairs and α^{-1} is the inverse distance. At this moment we discuss a cut-off version of (26.4.28) i.e. with $e_\varphi(.,.,.)$ and $P'_{\mu h,\varphi}(.)$. So, we have

$$C\mu^2 h^{-2}\bigl(1+\gamma_3^{-1}(h_2\gamma_3^{-\frac{1}{2}}\alpha^{-1})^s\bigr)^2\alpha^4.$$

Then integrating this expression with respect to $\alpha^{-1}\,d\alpha$ with $\alpha \le \gamma_3$ we arrive to $C\mu^2h^{-2}\bigl(\gamma_3^4 + h_2^2\gamma_3\bigr)$.

Therefore we conclude that

(26.4.29) A cut-off version of expression (26.4.28) with $\alpha = \alpha_3$ does not exceed $C\mu^2 h^{-2}\bigl(\gamma_3^4 + h_2^2\gamma_3\bigr)\alpha_2^3$

The first term here $C\mu^2 h^{-2}\gamma_3^4\alpha_2^3$ does not exceed $C\mu^2 h^{-2}\alpha_3^3$ (recall that $\alpha_j = \alpha_{j-1}\gamma_j$) and the summation over α_3-partition of 1-element returns $C\mu^2 h^{-2}$.

Consider the second term $C\mu^2 h^{-2} h_2^2\gamma_3\alpha_2^3$; its summation with respect to α_3-partition of α_2-element returns $C\mu^2 h^{-2}\alpha_2^3 h_2^2 \int \gamma_3^{-2}\, d\gamma_3 \lesssim C\mu^2 h^{-2}\alpha_2^3$ (really, recall that according to (26.4.14) $\gamma_3 \geq h_3^{\frac{2}{3}}$) and then the summation over α_2-partition of 1-element returns $C\mu^2 h^{-2}$.

Consider $B(x,\bar{\alpha}_2)$ and apply Fefferman–de Llave decomposition (26.3.8). There are two kinds of pairs:

(a) those with $|x-y| \geq \epsilon(\alpha_3(x) + \alpha_3(y))$ for all (x,y) and

(b) those with $|x-y| \leq \min(\alpha_3(x),\alpha_3(y))$ for all (x,y).

The total contribution of the pairs of the second type (i.e. summation is taken over *all* pairs of α_3-elements in $B(0,1)$) as we already know is $O(\mu^2 h^{-2})$. Meanwhile according to the analysis in the previous Subsection 26.4.2 a contribution of one pair of kind (a) does not exceed

$$C\underbrace{\bigl(h^{-2} + \mu h^{-1}\gamma_0^{-1}\gamma_1^{-1}\gamma_2^{-1}\gamma_3^{-1-\delta}\bar{\gamma}_3^{\delta}\bigr)\alpha_3^3}_{\text{at } x} \times \underbrace{\bigl(h^{-2} + \mu h^{-1}\gamma_0^{-1}\gamma_1^{-1}\gamma_2^{-1}\gamma_3^{-1-\delta}\bar{\gamma}_3^{\delta}\bigr)\alpha_3^3}_{\text{at } y} \times |x-y|^{-1}$$

where each of two first factors is just an estimate of the integral (26.4.24) calculated over corresponding domain. If we take the first term in the first factor and sum over α_3-partition of 1-element we get only the second factor multiplied by μh^{-1} and then summation was done in the previous subsection. Similarly we can deal with the first term in the second factor. On the other hand, if we take only second factors and sum over pairs of α_3-subelements of the same α_2-element we get

$$C\mu^2 h^{-2}\gamma_0^{-2}\gamma_1^{-2}\gamma_2^{-2}\alpha_2^5 \asymp C\mu^2 h^{-2}\alpha_2^3.$$

Then summation with respect to α_2-partition of 1-element returns $C\mu^2 h^{-2}$.

Consider now $B(\bar{x},\bar{\alpha}_1)$ and apply here Fefferman-de Llave decomposition (26.3.8). There are two kinds of pairs:

(a) those with $|x-y| \ge \epsilon(\alpha_2(x)+\alpha_2(y))$ for all (x,y) and

(b) those with $|x-y| \le \min(\alpha_2(x),\alpha_2(y))$ for all (x,y).

According to the above analysis the total contribution of the pairs of the second type (i.e. the summation is taken over *all* pairs of α_2-elements in $B(0,1)$) as we already know is $O(\mu^2h^{-2})$. Meanwhile according to the analysis in the previous Subsection 26.4.2 a contribution of one pair of kind (a) does not exceed

$$C\underbrace{\bigl(h^{-2}+\mu h^{-1}\gamma_0^{-1}\gamma_1^{-1}\gamma_2^{-1}\bigr)\alpha_3^3}_{\text{at } x}\times\underbrace{\bigl(h^{-2}+\mu h^{-1}\gamma_0^{-1}\gamma_1^{-1}\gamma_2^{-1}\bigr)\alpha_3^3}_{\text{at } y}\times|x-y|^{-1}$$

and here again we can "forget" about the first terms in each factor. Then the summation with respect to pairs of α_2-subelements of the same α_1-element results in $C\mu^2h^{-2}\gamma_0^{-2}\gamma_1^{-2}\alpha_1^5 \asymp C\mu^2h^{-2}\alpha_1^3$ where we avoid logarithmic factor in virtue of the same positive eigenvalue of $\operatorname{Hess} w$. Summation with respect to α_1-admissible partition of 1-element returns $C\mu^2h^{-2}$.

Consider now $B(\bar{x},\bar{\alpha}_0)$ and apply here Fefferman–de Llave decomposition. Again there are two kinds of pairs and the total contributions of the pairs of the second kind we already calculated and contribution of the pairs of α_1-subelements of the same 1-element does not exceed

$$C\mu^2h^{-2}\gamma_0^{-2}(1+|\log\hat{\gamma}_1|)^2\alpha_0^5 \lesssim C\mu^2h^{-2}(1+|\log\eta|)^2\alpha_0^3$$

and the summation with respect to α_0-partition of 1-element returns $C\mu^2h^{-2}(1+|\log\eta|)^2$.

Finally, consider $B(\bar{x},1)$ and apply here Fefferman-de Llave decomposition. Again there are two kinds of pairs and the total contributions of the pairs of kind (b) we already estimated while the total contribution of the pairs of kind (a) does not exceed $Ch^{-4}+C\mu^2h^{-2}\eta^{-1}(1+|\log\eta|)^2$ where we recalled the forgotten terms.

Again, this is estimate for cut-off expression. Going to uncut expression we repeat the same trick as before but as we deal with D-term we need to consider "mixed" pairs when one "factor" comes with θ and another with θ' but then contribution of such pair does not exceed $C(\nu h^{-4})^{\frac{1}{2}}(\nu' h^{-4})^{\frac{1}{2}}$. Easy details are left to the reader.

Therefore returning to the original scale we conclude that the contribution of ℓ-layer to (26.4.28) does not exceed

$$C\zeta^4\ell^3+CB^2\ell\zeta^{-1}(1+|\log\ell^2\zeta|)^2 \tag{26.4.30}$$

which is exactly the right-hand expression of (26.4.26) squared and multiplied by ℓ^{-1} due to scaling.

Remark 26.4.10. In comparison with the non-degenerate case $|\nabla W_B^{\mathsf{TF}}| \asymp \zeta^2\ell^{-1}$ we acquired the last term.

Assume first that condition (26.2.28) is fulfilled. Then

(i) For $B \leq Z^{\frac{4}{3}}$, $\ell \leq Z^{-\frac{1}{3}}$ we have $\zeta = Z^{\frac{1}{2}}\ell^{-\frac{1}{2}}$ and expression (26.3.42) returns $CZ^2\ell + CB^2\ell^{\frac{3}{2}}Z^{-\frac{1}{2}}$ and the summation with respect to ℓ results in its value as $\ell = Z^{-\frac{1}{3}}$ i.e. $CZ^{\frac{5}{3}} + CB^2Z^{-1}$ with the dominating first term.

(ii) For $B \leq Z^{\frac{4}{3}}$, $\ell \geq Z^{-\frac{1}{3}}$ we have $\zeta = \ell^{-2}$ and expression (26.3.42) returns $C\ell^{-5} + CB^2\ell^3$. We need to sum as long as $\mu h \leq 1$ i.e. $Z^{-\frac{1}{3}} \leq \ell \leq B^{-\frac{1}{4}}$ and the summation returns $CZ^{\frac{5}{3}} + CB^{\frac{5}{4}}$ with the dominating first term.

(iii) For $Z^{\frac{4}{3}} \leq B \leq Z^2$, $\ell \leq B^{-1}Z$ we have $\zeta = Z^{\frac{1}{2}}\ell^{-\frac{1}{2}}$ and expression (26.3.42) returns $CZ^2\ell + CB^2Z^{-\frac{1}{2}}\ell^{\frac{3}{2}}$. Then the summation results in $CZ^3B^{-1} + CB^{\frac{1}{2}}Z \lesssim Z^{\frac{3}{5}}B^{\frac{4}{5}}$.

Sure, we need to consider also mixed pairs of the layers and their contributions are

$$C\bigl(\zeta^2\ell^2 + CB\ell\zeta^{-\frac{1}{2}}(1+|\log \ell^2\zeta|)\bigr) \times \bigl(\zeta'^2\ell'^2 + CB\ell'\zeta'^{-\frac{1}{2}}(1+|\log \ell'^2\zeta'|)\bigr) \times (\ell+\ell')^{-1}$$

and the summation with respect to ℓ and ℓ' returns the same expression as above.

If assumption (26.2.28) is not fulfilled we use the same trick as in the previous Subsection 26.4.2. Therefore we arrive to the Statement (i) of Proposition 26.4.11 below. Applying the same arguments as in the proof of Proposition 26.4.9 we arrive to the Statement (ii):

Proposition 26.4.11. *(i) For $B \leq Z^2$ the contribution of the zone $\mathcal{X}_2 \times \mathcal{X}_2$ to expression* (26.4.28) *does not exceed $C\max(Z^{\frac{5}{3}}, Z^{\frac{3}{5}}B^{\frac{4}{5}})$.*

(ii) For $B \leq Z$ contribution of the zone $\mathcal{X}_2 \times \mathcal{X}_2$ to expression (26.4.28) *does not exceed $CZ^{\frac{5}{3}-\delta}$.*

26.4.4 Semiclassical T-Term

Semiclassical T-Term: Zone $\mathcal{X}_1$ Extended

First let us cover zone $\mathcal{X}_1$ extended.

What is $\mathcal{X}_1$ Extended? To define this zone $\mathcal{X}_1' := \{x\colon \ell(x)\le r\}$, where we define W using P rather than P_B let first us analyze the precise extension in the framework of N- and D-terms. For N-term we have approximation error and corresponding D-term not exceeding respectively $C(\mu h)^2\eta^{-\frac{1}{2}}h^{-3} = CB^2\zeta^{-\frac{3}{2}}\ell^2$ and this expression squared and multiplied by ℓ^{-1} i.e. $CB^4\zeta^{-3}\ell^3$. Finally, both expressions are summed to their values as $\ell = r$. Recall that either $\zeta = Z^{\frac{1}{2}}\ell^{-\frac{1}{2}}$ or $\zeta=\ell^{-2}$.

(i) Consider first $B\le Z^{\frac{4}{3}}$. Then we want these errors not to exceed respectively $CZ^{\frac{2}{3}}$ and $CZ^{\frac{5}{3}}$. Obviously, if $r\ge Z^{-\frac{1}{3}}$ the first condition is more restrictive. In this case plugging $\zeta = r^{-2}$ and we set $CB^2r^5 = Z^{\frac{2}{3}}$ i.e. $r = B^{-\frac{2}{5}}Z^{\frac{2}{15}}$. Then $r\ge Z^{-\frac{1}{3}}$ as long as $B\le Z^{\frac{7}{6}}$.

Then $\mu = Br^3 = B^{-\frac{1}{5}}Z^{\frac{6}{15}}\ge Z^{\frac{1}{6}}$ and $h = B^{-\frac{2}{5}}Z^{\frac{2}{15}}\ge Z^{-\frac{1}{3}}$; and one can see easily that $\mu\gtrsim h^{-\frac{1}{2}}$ provided $\ell(x)\ge r$.

(ii) Consider next $Z^{\frac{7}{6}}\le B\le Z^{\frac{4}{3}}$. Then for $r\le Z^{-\frac{1}{3}}$ we have $\zeta = Z^{\frac{1}{2}}r^{-\frac{1}{2}}$. In this case the second requirement is more restrictive and we set $B^4Z^{-\frac{3}{2}}r^{\frac{9}{2}} = Z^{\frac{5}{3}}$, i.e. $r = B^{-\frac{8}{9}}Z^{\frac{19}{27}}$. Then $\mu = B^{-\frac{1}{3}}Z^{\frac{5}{9}}$ and $h = Z^{-\frac{1}{2}}r^{-\frac{1}{2}} = B^{\frac{4}{9}}Z^{-\frac{23}{27}}$ and $\mu\ge h^{-\frac{3}{7}}$; this is better than $h^{-\frac{1}{3}}$.

However, we can do better than this: observe that $\mu h\le \eta$ if and only if $r\ge B^2Z^{-3}$ i.e. $B\le Z^{\frac{50}{39}}$, which is greater than $Z^{\frac{7}{6}}$ but less than $Z^{\frac{4}{3}}$, so we test μ and h in this case: $\mu = Z^{\frac{5}{39}}$ and $h = Z^{\frac{11}{39}}$ and $\mu\ge h^{-\frac{5}{11}}$ provided $\ell(x)\ge r$.

If $B\ge Z^{\frac{5}{11}}$ we will use another estimate for D-term: namely it does not exceed $(\mu h)^3h^{-6}r^{-1} = B^3r^5$ and we want it not to exceed $Z^{\frac{5}{3}}$, so $r = Z^{\frac{1}{3}}B^{-\frac{3}{5}}$ (which is still less than $Z^{-\frac{1}{3}}$) and $\mu = B^{\frac{1}{10}}$ and $h = B^{\frac{3}{10}}Z^{-\frac{2}{3}}$ and we test it as $B = Z^{\frac{4}{3}}$ when $\mu = B^{\frac{1}{10}}$ and $h = B^{-\frac{1}{5}}$, so exponent $-\frac{5}{11}$ fits again.

(iii) Finally, if $Z^{\frac{4}{3}}\le B\le Z^3$ then the error D-term does not exceed B^3r^5 and we want it not to exceed $B^{\frac{4}{5}}Z^{\frac{3}{5}}$. So, we pick up $r = B^{-\frac{11}{25}}Z^{\frac{3}{25}}$, $\mu = B^{\frac{17}{50}}Z^{-\frac{8}{25}}$, $h = B^{\frac{11}{50}}Z^{-\frac{14}{25}}$ and exponent $-\frac{5}{11}$ fits again.

When We can Use the same Method for T-Term? As far as semi-classical T-expression is concerned an approximation error of such approach in the localized and scaled settings is $C(\mu h)^{\frac{5}{2}}h^{-3}$ [27] which is $O(h^{-1})$ only

[27] If instead of $P_B(W)$ we use $P(W)+\frac{1}{2}P''(W)B^2$ rather than $P(W)$. This modification does not affect our previous arguments.

if $\mu \geq h^{-\frac{1}{5}}$. One can extend it to $\mu \geq h^{-\frac{1}{5}-\delta}$ using the same trick as in Remark 26.4.8 but we need to do better than this.

On the other hand, observe that in fact an approximation error does not exceed[27] $C(\mu h)^3\eta^{-\frac{1}{2}}h^{-3} \asymp CB^3\ell^2\zeta^{-\frac{7}{2}}$ in the localized scaled settings. The simple proof is left to the reader. This is translated into $CB^3\ell^2\zeta^{-\frac{3}{2}}$ into unscaled settings. Summation with respect to $\ell \leq r$ returns its value as $\ell = r$.

So we get CB^3r^5 as $B \leq Z^{\frac{4}{3}}$ and $r \geq Z^{-\frac{1}{3}}$. Consider first $B \leq Z$. In this case we want $CB^3r^5 \leq CZ^{\frac{5}{3}}$ and we pick up $r = B^{-\frac{3}{5}}Z^{\frac{1}{3}}$ which is greater than $Z^{-\frac{1}{3}}$ provided $B \leq Z^{\frac{10}{9}}$. Then $\mu = Br^3 = B^{-\frac{4}{5}}Z \geq Z^{\frac{1}{5}}$ and $h = r = B^{-\frac{3}{5}}Z^{\frac{1}{3}} \geq Z^{-\frac{4}{15}}$ and $\mu \geq h^{-\frac{3}{4}}$.

If $Z \leq B \leq Z^{\frac{4}{3}}$ but still $r \geq Z^{-\frac{1}{3}}$ we want $CB^3r^5 \leq CZ^{\frac{4}{3}}B^{\frac{1}{3}}$ [28] and we pick up $r = B^{-\frac{8}{15}}Z^{\frac{4}{15}}$ and we want it to be greater than $Z^{-\frac{1}{3}}$ i.e. $B \leq Z^{\frac{9}{8}}$. Then $\mu = Br^3 = B^{-\frac{3}{5}}Z^{\frac{4}{5}} \geq Z^{\frac{1}{8}}$ and $h = B^{-\frac{8}{15}}Z^{\frac{4}{15}} \geq B^{-\frac{1}{3}}$ and $\mu \geq h^{-\frac{3}{8}}$. It is not as good as $\mu \geq h^{-\frac{3}{7}}$.

Then we use the smooth canonical form. In the operator perturbation terms have factors μ^{-2}, μ^{-4} etc and we can use the standard approach to get rid of $\mu^{-4} \leq \mu h$, so we need to consider only μ^{-2}.

However let before scaling the second derivative of W be of magnitude θ; then after scaling it becomes of magnitude $\theta' = \gamma_0^2\gamma_1^2\theta$ and then the perturbation is of magnitude $\theta\mu^{-2}$ but contribution of the error will be (after we compare the true Riemann sum and the corresponding integral and their difference $Ch^{-3}\nu\mu^{-2}(\mu h)^2(\theta')^{-\frac{1}{2}} \times \alpha_1^3 \leq C\theta^{\frac{1}{2}}h^{-1}\gamma_0^{-1}\gamma_1^{-1}\alpha_1^3 \leq Ch^{-1}\gamma_1^{-\frac{1}{2}}\alpha_1^3$ where we used that $\theta \leq C\gamma_0^2\gamma_1$. Then summation over α_1-partition of α_0 element returns $Ch^{-1}\alpha_0^3$ and the summation over γ_0-partition returns Ch^{-1} as desired. Therefore we covered zone $\mathcal{X}_1$ for T-term.

Semiclassical T-Term: Zone $\mathcal{X}_2$

Tauberian eEstimate. Tauberian estimate for cut-off expression is rather simple:

$$C\mu h^{-1}\gamma_0^{-1}\gamma_1^{-1}\gamma_2^{-1} \times h\gamma_0^{-3}\gamma_1^{-\frac{5}{2}}\gamma_1^{-2} \times \gamma_0^4\gamma_1^3\gamma_2^2\alpha_2^3 \asymp C\mu\gamma_1^{-\frac{1}{2}}\gamma_2^{-1}\alpha_2^3$$

which nicely sums to $C\mu$ without logarithm due to the same positive eigenvalue arguments as before; for θ-cut-off with $\theta \geq \mu h$ we get the same albeit

[28] Because the semiclassical remainder estimate is not better than this. Actually, due to Remark 26.3.7 we can do marginally better than this, but we leave this analysis to the reader.

with γ_j defined by the same formula albeit with $(w_j - 2j\mu h s_j^{-1})$ replaced by θs_j^{-1} where s_j^{-1} means the scale; and this should be multiplied by $\theta/(\mu h)$. The result nicely sums to Ch^{-1}. This is what was required.

Magnetic Weyl Expression. Now we will get the same answer albeit $C\mu^{-4}$ term will be supplemented by $C\mu^{-\frac{3}{2}}h$ which in cut-off sum adds $C\mu^{-\frac{3}{2}}h \times \mu h^{-2} \le Ch^{-1}$.

We can use the standard approach, with an error $C\mu^{-\frac{3}{2}}h \times \theta/(\mu h) \times \mu h^{-2} \asymp C\theta\mu^{-\frac{3}{2}}h^{-2}$ which means that we can take $\theta = \mu^{\frac{3}{2}}h$ which is sufficient to deal with with $\theta \ge C\mu^{\frac{3}{2}}h$; in particular, for $\mu \ge h^{\frac{2}{3}}$ we are done. But for $\theta \ge \mu h^{1-\delta}$ we can apply the weak magnetic field approach, which is sufficient. So we arrive to inequality

$$|\int_{-\infty}^{\tau}\int \phi(x)\Bigl(e_\varphi(x,x,\tau) - P'_{\beta,\varphi}\bigl(w(x)+\tau\bigr)\Bigr)\,dx\,d\tau| \le Ch^{-1} \tag{26.4.31}$$

and therefore we arrive to

Proposition 26.4.12. *(i) If $B \le Z^2$ the contribution of zone $\mathcal{X}_2$ to the expression*

$$\int_{-\infty}^{\tau}\int \phi(x)\Bigl(e_\varphi(x,x,\tau) - P'_{B,\varphi}\bigl(W(x)+\tau\bigr)\Bigr)\,dx\,d\tau \tag{26.4.32}$$

does not exceed $C\max\bigl((Z+B)^{\frac{1}{3}}Z^{\frac{4}{3}}, Z^{\frac{3}{5}}B^{\frac{4}{5}}\bigr)$.

(ii) If $B \le Z$ the contribution of zone $\mathcal{X}_2$ to expression (26.4.32) *does not exceed $CZ^{\frac{5}{3}-\delta}$.*

Mollification Errors. Further, we need to estimate

$$\int \phi(x)\Bigl(P'_B(W(x)+\tau)) - P'_B(W_B^{\mathsf{TF}}(x)+\tau))\Bigr)\,dx, \tag{26.4.33}$$

$$\int \phi(x)\Bigl(P_B(W(x)+\tau)) - P_B(W_B^{\mathsf{TF}}(x)+\tau))\Bigr)\,dx, \tag{26.4.34}$$

$$\mathsf{D}\Bigl(\phi(x)\bigl(P'_B(W(x)+\tau)) - P'_B(W_B^{\mathsf{TF}}(x)+\tau))\bigr),\; \phi(x)\bigl(P'_B(W(x)+\tau)) - P'_B(W_B^{\mathsf{TF}}(x)+\tau))\bigr)\Bigr) \tag{26.4.35}$$

and

$$\|\phi(x)\nabla\bigl(W(x)-W_B^{\mathsf{TF}}(x)\bigr)\|^2. \tag{26.4.36}$$

We start from local versions (so in fact we dealing with w and w_β^{TF}).

Obviously after all rescalings $\hbar=h\gamma_0^{-3}\gamma_1^{-\frac{5}{2}}\gamma_2^{-2}$ and therefore $\varepsilon=\hbar^{\frac{3}{2}}=h^{\frac{3}{2}}(\gamma_0^{-3}\gamma_1^{-\frac{5}{2}}\gamma_2^{-2})^{-\frac{3}{2}}$ where we set $\delta=0$ but we will show that we have a reserve to set it as $\delta>0$ if we want to estimate (26.4.33) by h and (26.4.34)–(26.4.36) by h^2.

We claim that

$$|w-w_\beta^{\mathsf{TF}}|\leq C\varsigma:=C\beta\eta\bigl(\gamma_0^4\gamma_1^3\gamma_2^2\varepsilon\bigr)^{\frac{5}{2}}. \tag{26.4.37}$$

and

$$|\nabla(w-w_\beta^{\mathsf{TF}})|\leq C\varsigma_1:=C\beta\eta\bigl(\gamma_0^4\gamma_1^3\gamma_2^2\varepsilon\bigr)^{\frac{3}{2}}. \tag{26.4.38}$$

Indeed, it follows from equation (26.4.2).

Then the contribution of α_2-element to (26.4.34) does not exceed $C\varsigma\varepsilon\alpha_2^3$ as measure of zone of α_2-element where $w\neq w_\beta^{\mathsf{TF}}$ is $O(\varepsilon\alpha_2^3)$. One can see easily that $\varsigma\varepsilon=O(h^{\frac{7}{3}})$ and therefore $C\varsigma\varepsilon\alpha_2^3=O(h^{\frac{7}{3}}\alpha_2^3)$ and the summation over α_2-partition of 1-element returns $O(h^{\frac{7}{3}})$.

Modulo above calculations the contribution of α_2-element to (26.4.33) does not exceed $C\beta\varsigma^{\frac{1}{2}}\varepsilon\alpha_3^2$. One can check easily that $\varsigma\varepsilon=O(h^{\frac{3}{2}}\gamma_2^{-\frac{1}{2}})$ and therefore $C\varsigma^{\frac{1}{2}}\varepsilon\alpha_2^3=O(h^{\frac{7}{3}}\alpha_1^3\gamma_2^{\frac{5}{2}})$ and the summation over α_2-partition of α_1-element returns $O(h^{\frac{3}{2}}\alpha_1^3)$ and then the summation over α_1-partition of 1-element returns $O(h^{\frac{3}{2}})$.

Similarly, expression (26.4.35) with $\phi=\phi_{\alpha_2}$ does not exceed $C\varsigma\varepsilon_2\alpha_2^5\leq Ch^3\alpha_2^4$ and the summation over α_2-partition of 1-element returns $O(h^3)$. However we need to consider disjoint pairs of α_2-elements belonging to given α_1-element and their contribution does not exceed

$$Ch^3\int\gamma_{2x}^{-\frac{1}{2}}\gamma_{2y}^{-\frac{1}{2}}|x-y|^{-1}\,dxdy\leq Ch^2\alpha_1^5$$

and then summation over α_1-partition of 1-element returns $O(h^{\frac{3}{2}})$. We need also to consider disjoint pairs of α_1-elements belonging to given 1-element and their contribution does not exceed $Ch^3\int|x-y|^{-1}\,dxdy=O(h^3)$.

Finally, contribution of α_2-element to (26.4.36) does not exceed $C\varsigma_1^2\varepsilon\alpha_2^3$ and one can check easily that this does not exceed $C\alpha_1^3\gamma_2^{\frac{8}{3}}h^{\frac{8}{3}}$ and the summation over α_2-partition of α_1-element returns $C\alpha_1^3 h^{\frac{8}{3}}$; then summation over 1-partition of 1-element returns $O(h^{\frac{8}{3}})$.

So, the scaled versions of (26.4.33) and (26.4.34)–(26.4.36) do not exceed Ch and Ch^2 respectively. Then the original versions of (26.4.33), (26.4.34), (26.4.34), and (26.4.36) do not exceed respectively $C\zeta^3\ell^3\times(\zeta\ell)^{-1}=C\zeta^2\ell^2$, $C\zeta^5\ell^3\times(\zeta\ell)^{-2}=C\zeta^3\ell$, $C\zeta^6\ell^5\times(\zeta\ell)^{-2}=C\zeta^4\ell^3$, and $C\zeta^4\ell\times(\zeta\ell)^{-2}=C\zeta^2\ell^{-1}\le C\zeta^4\ell^3$.

Leaving the easy details to the reader we arrive to

Proposition 26.4.13. *(i) Contribution of zone $\mathcal{X}_2$ to the mollification error* (26.4.33) *does not exceed $CZ^{\frac{2}{3}}$.*

(ii) Contribution of zone $\mathcal{X}_2$ to the mollification error (26.4.34) *does not exceed $CZ^{\frac{5}{3}}+o(Z^{\frac{4}{3}}B^{\frac{1}{3}})$.*

(iii) Contributions of zone $\mathcal{X}_2$ to the mollification errors (26.4.35) *and* (26.4.36) *do not exceed $CZ^{\frac{5}{3}}$.*

and

Proposition 26.4.14. *Let $B\le Z$. Then*

(i) Contribution of zone $\mathcal{X}_2$ to the mollification error (26.4.33) *does not exceed $CB^\delta Z^{\frac{2}{3}-\delta}$.*

(ii) Contributions of zone $\mathcal{X}_2$ to the mollification errors (26.4.35)–(26.4.35) *do not exceed $CB^\delta Z^{\frac{5}{3}-\delta}$.*

Remark 26.4.15. Consider the mollification parameter in "absolute" scale (i.e. ℓ-scale): $\varepsilon=\gamma_0\gamma_1\gamma_2\gamma(h/\gamma_0^3\gamma_1^{\frac{5}{2}}\gamma_2^2)^{\frac{2}{3}-\delta}$. One can see easily that $\varepsilon\ge h^{\frac{2}{3}-\delta}\ge(\mu^{-1}h)^{\frac{1}{2}-\delta_1}$ which makes reduction possible.

Remark 26.4.16. All statements of Propositions 26.4.13 and 26.4.14 are valid for semiclassical errors as well except statements, concerning T-term; tose should include also terms $Ca^{-\frac{1}{2}}Z^{\frac{3}{2}}$ for $a\le Z^{-\frac{1}{3}}$ and $Ca^{-\delta}Z^{\frac{5}{3}+\frac{1}{3}\delta}$ for $a\ge Z^{-\frac{1}{3}}$.

26.4.5 Zone $\mathcal{X}_3$

Zone $\mathcal{X}_3$ defined by $\mu h\geq C_0$, $h\leq 1$, $\{x\colon \ell(x)\leq \epsilon_0\bar{r}\}$ appears only as $Z^{\frac{4}{3}}\leq B\leq Z^3$. In this zone W_B^{TF} is smooth and no mollification is necessary. Further, in this zone the canonical form contains only one number $j=0$ and $|D^\alpha W|\leq C_\alpha\zeta^2\ell^{-|\alpha|}$ and $W\asymp\zeta^2$.

Therefore we have non-degeneracy condition fulfilled and applying the standard theory we conclude that in the scaled version contribution of $B(0,1)$ to the semiclassical errors in N- and T-terms and into D-term are $C\mu h^{-1}$, $C\mu$ and $C\mu^2h^{-2}$ respectively.

In the unscaled version they become $CB\ell^2$, $CB\ell\zeta\leq CBZ^{\frac{1}{2}}\ell^{\frac{1}{2}}$ and $CB^2\ell^3$ and after summation (where for D-term we need to consider mixed contribution of different layers) we arrive to the same expressions calculated as $\ell=\bar{r}=B^{-\frac{2}{5}}Z^{\frac{1}{5}}$ i.e. $CB^{\frac{1}{5}}Z^{\frac{2}{5}}$, $CB^{\frac{4}{5}}Z^{\frac{3}{5}}$ and $CB^{\frac{4}{5}}Z^{\frac{3}{5}}$ respectively. Thus we have proven

Proposition 26.4.17. *Let $Z^{\frac{4}{3}}\leq B\leq Z^3$. Then*

(i) Contribution of zone $\mathcal{X}_3$ to the N-error does not exceed $CZ^{\frac{2}{5}}B^{\frac{1}{5}}$.

(ii) Contributions of zone $\mathcal{X}_3$ to the T-error and D-term do not exceed $CZ^{\frac{3}{5}}B^{\frac{4}{5}}$.

26.5 Semiclassical Analysis in the Boundary Strip for $M\geq 2$

To finish our analysis we need to get the same estimates as before in the *boundary strip*

$$\mathcal{Y}\coloneqq\{x\colon W(x)+\nu\leq\epsilon G,\ \epsilon\bar{r}\leq\ell(x)\leq c\bar{r}\}\tag{26.5.1}$$

with

$$G\coloneqq\begin{cases}(Z-N)_+^{\frac{4}{3}} & \text{for}\quad B\leq (Z-N)_+^{\frac{4}{3}},\\ B & \text{for}\quad (Z-N)_+^{\frac{4}{3}}\leq B\leq Z^{\frac{4}{3}},\\ Z^{\frac{4}{5}}B^{\frac{2}{5}} & \text{for}\quad B\geq Z^{\frac{4}{3}}.\end{cases}\tag{26.5.2}$$

which coincides with (26.2.41) as $B\geq (Z-N)^{\frac{4}{3}}$. Recall that $\bar{r}=(Z-N)_+^{-\frac{1}{3}}$, $\bar{r}=B^{-\frac{1}{4}}$ and $\bar{r}=B^{-\frac{2}{5}}Z^{\frac{1}{5}}$ in these three cases respectively. Analysis of the *external zone* $\mathcal{X}_4 := \{x\colon \ell(x) \ge C_1\bar{r}\}$ will be trivial and *inner zone* $\{x\colon W(x)+\nu \ge \epsilon G\}$ has been covered already.

26.5.1 Properties of W_B^{TF} if $N = Z$

Let us explore properties of W_B^{TF} in $\mathcal{Y}$ if $N = Z$ [29] Let us rescale $x \mapsto x' = x\bar{r}^{-1}$, $W \mapsto w = G^{-1}W$ and define $h = G^{-\frac{1}{2}}\bar{r}^{-1}$, $\mu = G^{-\frac{1}{2}}B\bar{r}$. Then

(a) In the case $B \le Z^{\frac{4}{3}}$ we need to rescale $w(x') = B^{-1}W_B^{\mathsf{TF}}(x'\bar{r})$ and take $h = B^{-\frac{1}{4}} \le 1$, $\mu = B^{\frac{1}{4}} \ge 1$, $\mu h = 1$.

(b) On the other hand, for $B \ge Z^{\frac{4}{3}}$ one should set $w(x') = \bar{r}Z^{-1}W_B^{\mathsf{TF}}(x'\bar{r})$ and $h = (Z\bar{r})^{-\frac{1}{2}} = (BZ^{-3})^{\frac{1}{5}} \le 1$, $\mu = BZ^{-\frac{1}{2}}\bar{r}^{\frac{3}{2}} = B^{\frac{2}{5}}Z^{-\frac{1}{5}} \ge 1$, $\mu h = B^{\frac{3}{5}}Z^{-\frac{4}{5}} \ge 1$ ($\mu h \asymp 1$ iff $B \lesssim Z^{\frac{4}{3}}$, $h \asymp 1$ iff $B \asymp Z^3$).

We will use now only rescaled coordinates unless the opposite is specified. Then in $\mathcal{Y}$ rescaled

$$\Delta w = \kappa w_+^{\frac{1}{2}}, \qquad \kappa = 12, \qquad w \to \theta = \nu\bar{\zeta}^{-2} \quad \text{as} \quad |x| \to \infty, \tag{26.5.3}$$

with $\bar{\zeta} := G^{\frac{1}{2}}$ where one can always get $\kappa = 12$ after rescaling $w \mapsto 144\kappa^{-2}w$.

Proposition 26.5.1. *Let $Z = N$. Then in $\mathcal{Y}$ after rescaling*

$$|D^\alpha w| \le C_\alpha w\gamma^{-|\alpha|} \qquad \forall\alpha \tag{26.5.4}$$

with the scaling function $\gamma = w^{\frac{1}{4}}$ and

$$|\nabla w^{\frac{1}{4}}| \le 1 + Cw^t \tag{26.5.5}$$

with some constant C and exponent $t > 0$.

Proof. (a) Rescaling $x \mapsto x\bar{r}^{-1}$ we get an equations $(26.5.3)_0$ = (26.5.3) with $\theta = 0$. We know that $W = 0$ for $\ell(x) \ge c\bar{r}$; so after rescaling $w = 0$ for $\ell(x) \ge c$. On the other hand, $w \asymp 1$ as $\ell(x) \le \epsilon$ (uniformly with respect to all the parameters).

Let us consider solution of the equation

$$\Delta w_s = 12 w_+^s \tag{26.5.6}$$

[29] I.e. $\nu = 0$ and $G = B\bar{r}^{-4}$.

in $\Omega = \{w \le \epsilon, \ell \le c\}$ with the boundary condition $w_s = w$ at $\partial\Omega$; $s > \frac{1}{2}$.

Note first that $w_s \geq 0$. Really, w_s is the solution of the variational problem to minimize

$$\|\nabla w\|^2 + 24(s+1)^{-1} \int w_+^{s+1}\, dx \tag{26.5.7}$$

and one makes this functional only less replacing w by w_+.

Further, the standard maximum principle arguments show that $w_s \searrow$ as $s \searrow$[30]. Obviously $w_s \searrow w$ and $w_s \to w$ in $\mathscr{C}^\infty$ in $\{x\colon w(x) > 0\}$ as $s \searrow \frac{1}{2}$.

We claim that

$$w_s \in \mathscr{C}^{4s+2}. \tag{26.5.8}$$

To prove (26.5.8) note first that $w \in \mathscr{C}^{2-\delta'}$ uniformly with respect to all the parameters for any $\delta' > 0$. Then $w_s^s \in \mathscr{C}^{s-\delta}$ and then (26.5.6) yields that $w_s \in \mathscr{C}^{2+s-\delta}$ as soon as $s - \delta \notin \mathbb{Z}$. Then since $w_s \geq 0$ we get $|\nabla w_s| \le c w_s^{\frac{1}{2}}$ and so $w_s^s \in \mathscr{C}^{s-\frac{1}{2}}$. Then equation (26.5.6) again yields that $w_s \in \mathscr{C}^{s+\frac{3}{2}}$.

Now we need more subtle arguments. First, for $|y| = 1$

$$w_s(x+ty) = w_s(x) + t(\nabla w_s)_x \cdot y + \frac{1}{2}(\nabla^2 w_s)_x(y)t^2 + O\bigl(t^3\bigr). \tag{26.5.9}$$

Then the lowest eigenvalue ς of $\nabla^2 w_s$ at x should be greater than $-Cw_s^{\frac{1}{3}}$. Indeed, otherwise we can take y as the corresponding eigenvector and t with $|t| = \epsilon\varsigma$ and with a sign making second term non-positive and get $w_s(x+ty) < 0$.

This lower estimate for eigenvalues of $\nabla^2 w_s$ and equation (26.5.6) yield that $|\nabla^2 w_s| \le Cw_s^{\frac{1}{3}}$. But then $|\nabla w_s| \le Cw_s^{\frac{2}{3}}$. Really, otherwise picking $y = |\nabla w_s|^{-1}\nabla w_s$ with $|t| = \epsilon |\nabla w_s|^{\frac{1}{2}}$ and an appropriate sign we would get $w_s(x+ty) < 0$.

These estimates yield that $w_s(x') \asymp w_s(x)$ in $B\bigl(x, \gamma(x)\bigr)$ with $\gamma(x) = \epsilon w_s^{\frac{1}{3}}$. Then $w_s^s \in \mathscr{C}^{\frac{3}{2}}$. In fact, let us consider $f = w_s^{s-1}\nabla w$ and $|f(x) - f(x')|$. Let

[30] If $\Delta w_i = f_i(w_i)$ in Ω, $f_i(w) \nearrow$ as $w \nearrow$ and $f_1(w) \ge f_2(w)$ then $\Delta(w_1 - w_2) > 0$ as $w_1 > w_2$ and then $w_1 - w_2$ does not reach maximum inside Ω.

us consider first $|x-x'|\ge \frac{1}{3}\bigl(\gamma(x)+\gamma(x')\bigr)$; since $|f(x)|\le \gamma(x)^{\frac{1}{2}}$ at each point we get that $|f(x)-f(x')\le |x-x'|^{\frac{1}{2}}$.

On the other hand, for $|x-x'|\le \frac{1}{3}\bigl(\gamma(x)+\gamma(x')\bigr)$ we conclude that $\gamma(x)\asymp\gamma(x')$ and $|f(x)-f(x')|\le |\nabla f|\cdot|x-x'|\le |x-x'|^s$ due to inequality $|\nabla f|\le |\nabla^2 w_s|w_s^{s-1}+|\nabla w_s|^2w_s^{s-2}\le C\gamma^{s-1}$.

Therefore $w_s^s\in\mathscr{C}^{s+1}$ and equation (26.5.6) yields that $w_s\in\mathscr{C}^{3+s}$.

(b) In the next round we assume that $w_s\in\mathscr{C}^{4+s-\delta}$ with *some* $\delta\in(0,1)$. Then

$$w_s(x+ty)\le w_s(x)+t(\nabla w_s)_x\cdot y+\frac{1}{2}(\nabla^2 w_s)_x(y)t^2+\frac{1}{6}(\nabla^3 w_s)_x(y)t^3+C|t|^p \tag{26.5.10}$$

with $p=\min(4,4+s-\delta)$.

We claim now that the lowest possible eigenvalue ς of $\bigl(\nabla^2 w_s\bigr)_x$ is greater than $-Cw_s^{(p-2)/p}$. Really, otherwise let us pick up y as the corresponding eigenvector, t with $|t|=\epsilon|\varsigma|^{1/(p-2)}$ and with a sign making expression

$$t(\nabla w_s)_x\cdot y+\frac{1}{6}t^3(\nabla^3 w_s)_x(y)$$

non-positive and get $w_s(x+ty)<0$ again. Now equation (26.5.6) yields that inequality

$$|\nabla^k w_s|\le Cw_s^{(p-k)/p} \tag*{(26.5.11)$_k$}$$

holds with $k=2$.

Further, we claim that this inequality holds with $k=1,3$. Indeed, if one or both of these inequalities are violated then let us take corresponding y and t with

$$|t|=\epsilon\Bigl(|\nabla w_s|^{1/(p-1)}+|\nabla^3 w_s(y)|^{1/(p-3)}\Bigr)$$

(calculated on y); replacing ϵ by 2ϵ if necessary we get

$$\bigl|t(\nabla w_s)_x\cdot y+\frac{1}{6}t^3(\nabla^3 w_s)_x(y)\bigr|\ge \epsilon_0|t(\nabla w_s)_x\cdot y|+|\frac{1}{6}t^3(\nabla^3 w_s)_x(y)|$$

and choosing an appropriate sign of t we get $w(x+ty)<0$.

Therefore inequalities $(26.5.11)_{1-3}$ *hold*. The same arguments as above with $\gamma = w_s^{1/p}$ lead us to $w^s \in \mathscr{C}^{ps}$ and then equation (26.5.6) yields that $w_s \in \mathscr{C}^{ps+2}$. So, now we came back with δ replaced by $\delta' = 2 + s - ps$ and one can see easily that if $\delta > s$ then $\delta' = s + (2 - 4s) + (\delta - s)s$ and after few repeats $\delta < s$. Then we get (26.5.8). Unfortunately, constants depend on s due to the fact that $\Delta w \in \mathscr{C}^2$ fails to yield $w \in \mathscr{C}^4$.

(c) Now we are going to finish the proof of (26.5.4). Let us consider w_s again and let $\gamma = \gamma_{s,\delta} = w_s^{1/(4-\delta)}$. Due to the previous inequalities $\gamma \in \mathscr{C}^1$. We claim that $|\nabla\gamma|$ is bounded uniformly with respect to s, δ. Note first that $\Delta\gamma^{4-\delta} = \gamma^{(4-\delta)s}$ implies that

$$a|\nabla\gamma|^2 + b\gamma\Delta\gamma = \gamma^\sigma \tag{26.5.12}$$

with $a = \frac{1}{12}(4-\delta)(3-\delta)$, $b = \frac{1}{12}(4-\delta)$, and $\sigma = 4s - 2 + (1-s)\delta$. Let $\psi = |\nabla\gamma|^2$; obviously ψ is uniformly bounded at $\partial\Omega$. Let us consider maximum of ψ reached inside Ω. At the point of maximum

$$\sum_i \gamma_{x_ix_j}\gamma_{x_i} = 0 \tag{26.5.13}$$

and

$$\frac{1}{2}\Delta\psi = \sum_{i,j}\gamma^2_{x_ix_j} + \sum_i \gamma_{x_i}\bigl(\Delta\gamma\bigr)_{x_i} = \\ \sum_{i,j}\gamma^2_{x_ix_j} + b^{-1}\sum_i \gamma_{x_i}\Bigl(\gamma^{-1}\bigl(\gamma^\sigma - a|\nabla\gamma|^2\bigr)\Bigr)_{x_i}.$$

Due to (26.5.12) and due to (26.5.13) this expression is equal to

$$\sum_{i,j}\gamma^2_{x_ix_j} - b^{-1}\gamma^{-2}|\nabla\gamma|^2\bigl(\gamma^\sigma - a|\nabla\gamma|^2\bigr) + b^{-1}\sigma\gamma^{\sigma-2}|\nabla\gamma|^2$$

and therefore at an inner point of minimum $a|\nabla\gamma|^2 \leq \gamma^\sigma$. So, $|\nabla\gamma| \leq C$ is proven and for $s \searrow \frac{1}{2}$, $\delta \searrow 0$ we get that $|\nabla w^{\frac{1}{4}}| \leq C$.

Let us pick $\gamma(x) = \epsilon' w^{\frac{1}{4}}(x)$; then $|\nabla w| \leq \frac{1}{2}$ and $w(x) \asymp w(\mathrm{x})$ in $B\bigl(x, \gamma(\mathrm{x})\bigr)$. This and equation (26.5.6) easily yield (26.5.4).

To prove inequality (26.5.5) let us consider w_s again and let us take now $\psi = |\nabla\gamma|^2 - F\gamma^{2t}$ with $t > 0$; obviously ψ is non-positive at $\partial\Omega$ for sufficiently large F. Let us consider maximum of ψ reached inside Ω. At the point of maximum

$$\sum_i \gamma_{x_ix_j}\gamma_{x_i} - Ft\gamma^{2t-2}\gamma_{x_j} = 0 \tag{26.5.13$'$}$$

and the same arguments as before (plus inequality $|\nabla\gamma| \le C_0$) show that at an inner point of maximum $a|\nabla\gamma|^2 \le \gamma^\sigma + CtF\gamma^{2t}$ where C does not depend on F and small $t>0$. Then at this point $\psi\le 1$ for small enough $t>0$ and as $s\to\frac{1}{2}$ and $\delta\to 0$ we get (26.5.5). □

The following statement heavily uses estimate (26.5.5):

Proposition 26.5.2. *The following estimate holds*

$$\mathsf{D}(\gamma^{-1+s},\gamma^{-1+s}) \le Cs^{-2} \tag{26.5.14}$$

with some constant C which does not depend on $s\in(0,1)$ where we set $\gamma^{-1+s} := w_+^{\frac{1}{4}(-1+s)}$ (i.e. it is 0 as $w\le 0$).

Proof. As in the notations of the proof of Proposition 26.5.1 $\delta = 0$ and $s=\frac{1}{2}$ we have (26.5.12) with $a=1$, $b=3$ and $\sigma=0$:

$$\frac{1}{3}\gamma\Delta\gamma + |\nabla\gamma|^2 = 1. \tag{26.5.15}$$

Then

$$\gamma^{-1+s} = \gamma^{-1+s}|\nabla\gamma|^2 + \frac{1}{3}\gamma^s\Delta\gamma = (1-\frac{s}{3})\gamma^{-1+s}|\nabla\gamma|^2 + \frac{1}{3(1+s)}\Delta\gamma^{1+s}$$

and

$$\mathsf{D}(\gamma^{-1+s},\gamma^{-1+s}) \le (1-\frac{s}{3})\mathsf{D}(\gamma^{-1+s}|\nabla\gamma|^2,\gamma^{-1+s}) + C \le \\ (1-\frac{s}{3})\mathsf{D}(\gamma^{-1+s},\gamma^{-1+s}) + C\mathsf{D}(\gamma^{-1+t+s},\gamma^{-1+s}) + C$$

due to (26.5.5) and this yields

$$\mathsf{D}(\gamma^{-1+s},\gamma^{-1+s}) \le Cs^{-2}\mathsf{D}(\gamma^{-1+t+s},\gamma^{-1+t+s}) + Cs^{-1}.$$

Substituting $s+mt$ instead of s, $0\le m\le Ct^{-1}$ we recover (26.5.14). □

26.5.2 Analysis in the Boundary Strip $\mathcal{Y}$ for $N \geq Z$

We consider now the case of if $N \geq Z$ (i.e. $\nu = 0$ and $G = B\bar{r}^{-4}$).

It is really easy to construct the proper potential in this case: we just take

$$w_\varepsilon = w\phi_\varepsilon, \qquad \phi_\varepsilon = f(w\varepsilon^{-4}) \tag{26.5.16}$$

with $f \in \mathscr{C}^\infty((\frac{1}{2},\infty))$, $\operatorname{supp}(f) \subset (\frac{1}{2},\infty)$, $0 \leq f \leq 1$, $f(t) = 1$ for $t > 1$. Note that due to (26.5.3)

$$\begin{aligned}
&\mathsf{D}(\gamma^{-1}\phi_\varepsilon, \gamma^{-1}\varphi_\varepsilon) \leq C\varepsilon^{-2s}\mathsf{D}(\gamma^{s-1},\gamma^{s-1}) \leq Cs^{-2}\varepsilon^{-2s},\\
&\mathsf{D}(1-\phi_\varepsilon, 1-\phi_\varepsilon) \leq C\varepsilon^{2-2s}\mathsf{D}(\gamma^{s-1},\gamma^{s-1}) \leq Cs^{-2}\varepsilon^{2-2s};
\end{aligned}$$

then minimizing with respect to s $(= |\log\varepsilon|^{-1})$ the right-hand expression we conclude that

$$\mathsf{D}\bigl(\gamma^{-1}\phi_\varepsilon, \gamma^{-1}\varphi_\varepsilon\bigr) + \varepsilon^{-2}\mathsf{D}\bigl(1-\phi_\varepsilon, 1-\phi_\varepsilon\bigr) \leq C\bigl(1+|\log\varepsilon|\bigr)^2 \tag{26.5.17}$$

and therefore

$$\int \gamma^{-1}\phi_\varepsilon\,dx + \varepsilon^{-1}\int (1-\phi_\varepsilon)\,dx \leq C\bigl(1+|\log\varepsilon|\bigr). \tag{26.5.18}$$

Remark 26.5.3. (i) Recall that all these integrals are taken over domain $\{x\colon w(x) > 0\}$. To avoid possible troubles we pick $\varepsilon = h^{\frac{1}{3}}$ and set in the zone $\{x\colon w(x) \leq C_0 h^{\frac{4}{3}}\}$

$$\gamma(x) = \operatorname{dist}(x, \{w \geq 2C_0h^{\frac{4}{3}}\}),$$

$$w_\varepsilon = \begin{cases} -\gamma^4\phi'_\varepsilon & \text{for } \gamma \leq \varepsilon,\\ -\varepsilon^4 & \text{for } \gamma \geq \varepsilon \end{cases} \tag{26.5.16$'$}$$

with $\phi'_\varepsilon = f(\gamma\varepsilon^{-1})$ and then in the complemental domain $\{x\colon w(x) \leq -\varsigma^2\}$ our assumptions are fulfilled with $\varsigma = \varepsilon^2$ and $\varsigma\gamma = \gamma^3 \geq h$.

(ii) Further, for $\varepsilon = h^{\frac{1}{3}-\delta}$ with sufficiently small exponent $\delta > 0$ it does not break estimate for mollification error in T-term.

(iii) Furthermore, for $t > \varepsilon$

$$\operatorname{mes}(\{x\colon \gamma(x) \leq t\}) \leq Ct^3\varepsilon^{-3}\operatorname{mes}(\{x\colon \gamma(x) \leq \epsilon\varepsilon\})$$

and therefore

$$h^s\int \gamma^{-1-s}\varsigma^{-s}\,dx\le C\varepsilon^{-1}\operatorname{mes}(\{x\colon \gamma(x)\le \epsilon\varepsilon\})\le CL:=C(1+|\log h|)$$

for sufficiently large s.

Using these estimates and the last remark we can prove easily

Proposition 26.5.4. *Let $N\ge Z$. Then*

(i) Contribution of $\mathcal{Y}\cup\mathcal{X}_4$ with external zone $\mathcal{X}_4:=\{x\colon w(x)=0\}$ *to mollification and semiclassical errors in* N*-term do not exceed* $CT_0\varepsilon^3(1+|\log\varepsilon|)$ *and* $R_0(1+|\log\varepsilon|)$ *respectively with*

$$T_0=B^{\frac{3}{4}},\qquad R_0=B^{\frac{1}{2}},\qquad T=B^{\frac{7}{4}},\qquad R=B^{\frac{5}{4}}\qquad \text{for}\ \ B\le Z^{\frac{4}{3}} \tag{26.5.19$_1$}$$

and

$$T_0=Z,\qquad R_0=B^{\frac{1}{5}}Z^{\frac{2}{5}},\qquad T=Z^{\frac{9}{5}}B^{\frac{2}{5}},\qquad R=Z^{\frac{3}{5}}B^{\frac{4}{5}}\qquad \text{for}\ \ Z^{\frac{4}{3}}\le B\le Z^3. \tag{26.5.19$_2$}$$

(ii) Contribution of $\mathcal{Y}\cup\mathcal{X}_4$ to mollification and semiclassical D*-terms do not exceed* $CT\varepsilon^6(1+|\log\varepsilon|)^2$ *and* $R(1+|\log\varepsilon|)^2$ *respectively.*

(iii) Contribution of $\mathcal{Y}\cup\mathcal{X}_4$ to both mollification and semiclassical errors in T*-term do not exceed* $CT\varepsilon^7(1+|\log\varepsilon|)$ *and* CR *respectively.*

Proof. Really, estimates for mollification errors and terms immediately follow from the inequality

$$\operatorname{mes}(\{x\colon w(x)\le\varepsilon^4\})\le C\varepsilon(1+|\log\varepsilon|) \tag{26.5.20}$$

which is due to (26.5.18).

Let us consider semiclassical errors and terms.

(i) Let us consider N-term first. Let us consider all possible balls and their contributions: the contribution of each ball $B\bigl(x,\gamma(x)\bigr)$ to the semiclassical error does not exceed $C\mu h^{-1}\gamma^2\asymp CB\bar{r}^2\gamma^2$ and the total contribution does not exceed

$$CR_0\int\gamma(x)^{-1}\,dx\le CR_0\bigl(1+|\log\varepsilon|\bigr) \tag{26.5.21}$$

where $R_0=B\bar{r}^2$; recall that $\gamma(x)\ge\varepsilon$.

(ii) Consider semiclassical D-term. Let us consider all possible balls and their contributions: the similar arguments with the analysis of disjoint balls of different types and with analysis of the intersecting balls (of the same type) lead us to the proper estimate of the contribution of $\mathcal{Y}_4 \cup \mathcal{X}_4$ to semiclassical D-term: namely, it does not exceed $CR_0^2\bar{r}^{-1}\bigl(1+|\log\varepsilon|\bigr)^2$ (i.e. expression (26.5.21) squared and multipled by $C\bar{r}^{-1}$) where $R_0^2\bar{r}^{-1} \asymp R$.

(iii) Consider T-term. Let us consider all possible balls and their contributions. Contribution of each ball $B\bigl(x,\gamma(x)\bigr)$ to the semiclassical error does not exceed $C\bar{\zeta}^2\mu\varsigma^2\gamma \asymp CB\bar{\zeta}^2\bar{r}\varsigma\gamma^2$ and the total contribution does not exceed

$$CR\int \varsigma(x)\gamma(x)^{-2}\,dx \asymp CR \tag{26.5.22}$$

where $R = B\bar{\zeta}^2\bar{r}$ and $\varsigma(x) \asymp \gamma(x)^2$. □

Then picking appropriate $\varepsilon = h^{\frac{1}{3}}$ we arrive to

Corollary 26.5.5. *Let $N \geq Z$. Then*

(i) Contributions of $\mathcal{Y} \cup \mathcal{X}_4$ to all errors in N*-terms do not exceed CR_0L with $L = (1+|\log BZ^{-3}|)$.*

(ii) Contribution of $\mathcal{Y} \cup \mathcal{X}_4$ to all D*-terms do not exceed CRL^2.*

(iii) Contribution of $\mathcal{Y} \cup \mathcal{X}_4$ to all errors in T*-terms do not exceed CR.*

We will sum contributions of all zones to errors in Propositions 26.5.14 and 26.5.17 below.

Remark 26.5.6. Could we get rid of the logarithmic factors i.e. make $L = 1$ as it was in the case $M = 1$?

(i) With the mollification errors we need to replace (26.5.20) by

$$\operatorname{mes}(\{x\colon w(x) \leq \varepsilon^4\}) \leq C\varepsilon; \tag{26.5.23}$$

(ii) With the semiclassical terms our arguments here are insufficient even if we established (26.5.23); we need extra propagation arguments in the direction of decaying w along magnetic lines–exactly as in the case $M = 1$. Surely there could be points where such arguments do not work; f.e. consider

$M=2$ and nuclei so that $|\mathsf{y}_1-\mathsf{y}_2|$ is slightly less than $\bar{r}_1+\bar{r}_2$ where $\bar{r}_{1,2}$ are precise radii of support. Then w reaches its minimum at $\mathcal{Y}$.

So, we need to prove that the measure of such points is sufficiently small (f.e. less than $C|\log BZ^{-3}|^{-1}$).

Unfortunately, we do not know how to make the above remark work and we suggest

Problem 26.5.7. Follow through the discussed plan. For $M=2$ it could be easier due to the rotational symmetry of the potential W_B^{TF}.

26.5.3 Analysis in the Boundary Strip $\mathcal{Y}$ for $N<Z$

Now let us consider the case of $N<Z$ (i.e. $\nu<0$).

Case $B\ge (Z-N)_+^{\frac{4}{3}}$

We start from the case $B\ge (Z-N)_+^{\frac{4}{3}}$ when $\bar{r}=\min(B^{-\frac{1}{4}},Z^{\frac{1}{5}}B^{-\frac{2}{5}})$ matching cases $B\lesssim Z^{\frac{4}{3}}$ and $Z^{\frac{4}{3}}\lesssim B\lesssim Z^3$.

Remark 26.5.8. (i) The results of the previous Subsection 26.4.2 remain true as long as $|\nu|G^{-1}\le C_0h^{\frac{4}{3}}$; in other words, as $(Z-N)_+\le C_0G\bar{r}h^{\frac{4}{3}}$. Plugging $\bar{r}$, G and h, we rewrite it as

$$(Z-N)_+\le C_0\min\bigl(B^{\frac{5}{12}},\,Z^{\frac{1}{5}}B^{\frac{4}{15}}\bigr) \tag{26.5.24}$$

matching cases $B\lesssim Z^{\frac{4}{3}}$ and $Z^{\frac{4}{3}}\lesssim B\lesssim Z^3$.

(ii) Therefore in this Subsection we assume that condition (26.5.24) fails. Let $\theta=|\nu|G^{-1}\asymp (Z-N)_+\cdot\max\bigl(B^{-\frac{3}{4}},\,Z^{-1}\bigr)$, also matching cases $B\lesssim Z^{\frac{4}{3}}$ and $Z^{\frac{4}{3}}\lesssim B\lesssim Z^3$.

Proposition 26.5.9. *Consider dependence of $W_B^{\mathsf{TF}}=W_{B(\nu)}^{\mathsf{TF}}(x)$ on ν. Then*

(i) $W_{B(\nu)}^{\mathsf{TF}}(x)+\nu$ is non-decreasing with respect to ν at each point x.

(ii) $W_{B(\nu)}^{\mathsf{TF}}(x)$ is non-increasing with respect to ν at each point x.

(iii) In particular, $W_{B(\nu)}^{\mathsf{TF}}(x)+\nu\nearrow W_{B(0)}^{\mathsf{TF}}(x)$ and $W_{B(\nu)}^{\mathsf{TF}}(x)\searrow W_{B(0)}^{\mathsf{TF}}(x)$ at each point x as $\nu\nearrow 0$.

Proof. (i) Consider $W_j := W^{\mathsf{TF}}_{B(\nu_j)} + \nu_j$ with $0 > \nu_1 > \nu_2$. One can prove easily that $W^{\mathsf{TF}}_B - V$ is a continuous function and since

$$W_1 - W_2 \to \nu_1 - \nu_2 \qquad \text{as} \quad \ell(x) \to \infty \tag{26.5.25}$$

with $\nu_1 - \nu_2 > 0$ we conclude that $W_1 \geq W_2$ at each point x (which is exactly our Statement (i)) unless $W_1 - W_2$ achieves a negative minimum at some point x^*:

(a) Let $x^* \neq \mathsf{y}_m$; then $\Delta(W_1 - W_2)(x^*) = P'_B(W_1) - P'_B(W_2) \leq 0$ because $W_1 < W_2$ at x^* and therefore x^* cannot be such point.

(b) Let $x^* = \mathsf{y}_m$. From Thomas-Fermi equations for $W_{1,2}$ one can prove easily that

$$(W_1 - W_2)(x) = (W_1 - W_2)(\mathsf{y}_m) + L_m(x - \mathsf{y}_m) + \\ \kappa_m |x - y_m|^{\frac{3}{2}} (W_1 - W_2)(\mathsf{y}_m) + O(|x - \mathsf{y}_m|^2)$$

near y_m where $L_m(x)$ is a linear function and $\kappa_m > 0$ and therefore if $(W_1 - W_2)(\mathsf{y}_m) < 0$, y_m cannot be a minimum point either.

(ii) So, $W_1 \geq W_2$ and therefore $\Delta(W_1 - W_2)(x^*) = P'_B(W_1) - P'_B(W_2) \geq 0$ and $W_1 - W_2$ is a subharmonic function. Then due to (26.5.25) we conclude that $W_1 - W_2 \leq \nu_1 - \nu_2$ i.e. $W^{\mathsf{TF}}_{B,(\nu_1)} \leq W^{\mathsf{TF}}_{B,(\nu_2)}$ at each point.

(iii) Statement (iii) follows from Statements (i) and (ii). □

From Statements (i) and (iii) we conclude immediately that

Corollary 26.5.10. *(i) $\rho^{\mathsf{TF}}_{B(\nu)}(x)$ is non-decreasing with respect to ν at each point x.*

(ii) $\rho^{\mathsf{TF}}_{B(\nu)}(x) \nearrow \rho^{\mathsf{TF}}_{B(0)}(x)$ at each point x as $\nu \nearrow 0$.

Therefore in the zone $\{x \in \mathcal{Y}\colon W^{\mathsf{TF}}_{B(\nu)} \geq (1+\epsilon)|\nu|\}$ we can apply the same (γ, ς) scaling with $\varsigma = \gamma^2$ defined for $\nu = 0$. Indeed, we know that there $W^{\mathsf{TF}}_{B(\nu)} + \nu \asymp W^{\mathsf{TF}}_{B(0)} \asymp \varsigma^2$ and $\varsigma = \gamma^2$.

Then Thomas-Fermi equation (26.2.3) implies that

$$|\nabla^\alpha W^{\mathsf{TF}}_{B(\nu)}| \leq C_\alpha \varsigma^2 \gamma^{-|\alpha|} \qquad \forall \alpha \tag{26.5.26}$$

and then we arrive to the Statement (i) in Proposition 26.5.11 below. On the other hand, in the zone $\{x\colon W^{\mathsf{TF}}_{B(\nu)}\le (1-\epsilon)|\nu|\}$ we can apply the same arguments but this zone is classically forbidden and we arrive to Statement (ii) below. In both cases $\varsigma\gamma\ge h$ (where in the latter case γ is the distance from x to $W^{\mathsf{TF}}_{B(\nu)}$ (scaled) and $\varsigma=|\theta|^{\frac{1}{2}}$ in virtue of Remark 26.5.8.

Proposition 26.5.11. *Let either $B\le Z^{\frac{4}{3}}$ and $|\nu|^{\frac{3}{4}}\ge Z^{\frac{2}{3}}$ or $Z^{\frac{4}{3}}\le B\le Z^3$ and $|\nu|^{\frac{3}{4}}\ge B^{\frac{1}{2}}$. Then*

(i) Contributions of zone $\{x\colon W^{\mathsf{TF}}_B(x)\ge (1+\epsilon_0)|\nu|\}$ to the semiclassical errors in N- and T-terms and into semiclassical D-term do not exceed CR_0L, CR and CRL^2 respectively.

(ii) Contributions of zone $\{x\colon W^{\mathsf{TF}}_B(x)\le (1-\epsilon_0)|\nu|\}$ to the semiclassical errors in N- and T-terms and into semiclassical D-term do not exceed CR_0L, CR and CRL^2 respectively.

Remark 26.5.12. Here actually we can replace L by $L_*=1+|\log\theta|$ with

$$\theta=|\nu|G^{-1}\asymp\begin{cases}(Z-N)_+B^{-\frac{3}{4}} & \text{if } (Z-N)_+^{\frac{4}{3}}\le B\le Z^{\frac{4}{3}},\\ (Z-N)_+Z^{-1} & \text{if } Z^{\frac{4}{3}}\le B\le Z^3;\end{cases}\tag{26.5.27}$$

Therefore we need to explore the following zone

$$\mathcal{Y}^*:=\{x\colon (1-\epsilon_0)|\nu|\le W^{\mathsf{TF}}_B(x)\le (1+\epsilon_0)|\nu|\}$$

in the framework of Proposition 26.5.11. In virtue of Remark 26.5.8 $\hbar\lesssim 1$ where

$$\hbar=h\theta^{-\frac{3}{4}}\asymp\begin{cases}(Z-N)_+^{-\frac{3}{4}}B^{\frac{5}{16}} & \text{if } B\le Z^{\frac{4}{3}},\\ (Z-N)_+^{-\frac{3}{4}}Z^{\frac{3}{20}}B^{\frac{1}{5}} & \text{if } Z^{\frac{4}{3}}\le B\le Z^3.\end{cases}\tag{26.5.28}$$

Let us rescale the ball $B(.,\alpha)$ to $B(.,1)$ by $x\mapsto x\alpha^{-1}$ with $\alpha=\theta^{\frac{1}{4}}$ (after we already rescaled $x\mapsto x\bar{r}^{-1}$). After this let us introduce scaling function γ_0 by (26.4.3). Then let us introduce consequently scaling functions γ_1 by (26.4.7), γ_2 by (26.4.13) and γ_3 by (26.4.14) [31)].

Consider contributions of different balls in this hierarchy into semiclassical and approximation errors in N- and T-terms and into D semiclassical and approximation D-terms.

[31)] With $j=\bar{j}=0$ and corrected as in $(26.4.3)^*$ and $(26.4.7)^*$.

(i) Consider first semiclassical error in N-term. Due to Chapter 18 the contribution of α_j element does not exceed $CB\ell_j^2 = CB\bar{r}^2\alpha_j^2$ for $j = 3, 2$, where recall that $\alpha_j = \gamma_0 \cdots \gamma_j$.

Then for $j = 2$ we have $CB\bar{r}^2\alpha_2^2 = CB\bar{r}^2\alpha_1^2\gamma_1^2$ and therefore we estimate the contribution of α_1 element by $CB\bar{r}^2\alpha_1^2 \int \gamma_2^{-1}\, dx$ [32], which also results in $CB\bar{r}^2\alpha_1^2$ but with the logarithmic factor. However we can get rid of this factor due to a simple observation:

(26.5.29) If $\gamma_2 \leq \epsilon$ then $\mathsf{Hess}(w_1)$ has at least two eigenvalues of magnitude 1 due to $|\Delta w_1| \leq \epsilon_1$.

Then the contribution of α_0 element does not exceed $CB\bar{r}^2\alpha_0^2 \int \gamma_1^{-1}\, dx$ [32]; we claim that it is $CB\bar{r}^2\alpha_0^2$. Indeed, we need to consider only points with $\gamma_1 \leq \epsilon$ and there we use a similar observation:

(26.5.30) If $\gamma_1 \leq \epsilon$ then $|\nabla^3 w'| \asymp 1$ and also $|\nabla^3 w' - e\otimes e\otimes e| \geq c^{-1}$ for any $e \in \mathbb{R}^3$ due to $|\partial_j \Delta w_1| \leq \epsilon_1$; here $\nabla^3 w'$ is a 3-tensor of the third derivatives of w'.

Further, the contribution of α element does not exceed $CB\bar{r}^2\alpha^2 \int \gamma_0^{-1}\, dx$ [32]; since $\gamma \geq \bar{\gamma}_0 = \hbar^{\frac{1}{3}}$, we estimate it by $CB\bar{r}^2\alpha^2\hbar^{-\frac{1}{3}}$.

Finally, since $\bar{r}^{-1}\mathcal{Y}^*$ is covered by no more than $CL_*\alpha^{-2}$ such elements[33], we conclude that

(26.5.31) The total contribution of $\mathcal{Y}^*$ into the semiclassical (and also approximation) errors in N-term does not exceed $CB\bar{r}^2\hbar^{-\frac{1}{3}}L_*$, where $L_* := (1 + |\log\theta|)$.

Plugging values of $\hbar$ and θ, we arrive to expression (26.5.33) in Proposition 26.5.13(i) below.

(ii) Similarly, in virtue of Subsubsection *26.3.1.2. Semiclassical* D*-Term* we know the that the contribution of the non-disjoint pair of α_j-elements to the semiclassical D-term does not exceed $CB^2\ell^3 = CB^2\bar{r}^3\alpha_j^3$ for $j = 3, 2$.

[32] With the integral calculated in the scaled coordinates.
[33] Indeed, due to Subsection 26.5.1 $\mathsf{mes}(\bar{r}^{-1}\mathcal{Y}^*) \leq C\alpha L_*$.

Therefore the contribution of all non-disjoint pairs of α_2 subelements to the same expression for α_1 element does not exceed $CB^2\bar{r}^3\alpha_1^3$. Adding all disjoint pairs, we get[32)]

$$CB^2\bar{r}^3\alpha_1^3 \iint |x-y|^{-1}\gamma_2(x)^{-1}\gamma_2(y)^{-1}\,dxdy. \tag{26.5.32}$$

Then using the results of Part (i) together with observation (26.5.29) we arrive to $CB^2\bar{r}^3\alpha_1^3$. So, contribution of the non-disjoint pair of α_1-elements to the semiclassical D-term does not exceed $CB^2\ell^3 = CB^2\bar{r}^3\alpha_1^3$.

Further, continuing in the same manner, we estimate the contribution of the non-disjoint pair of α_0-elements by $CB^2\bar{r}^3\alpha_0^3$.

Furthermore, in the same manner we estimate the contribution of the non-disjoint pair of α-elements by expression (26.5.32) with γ_2 replaced by γ_0, which does not exceed $CB^2\bar{r}^3\alpha^3\hbar^{-\frac{2}{3}}$.

Finally, adding contribution of all non disjoint pairs and using results of Part (i), we conclude that the total contribution of $\mathcal{Y}^*\times\mathcal{Y}^*$ into the semiclassical (and also approximation) D-terms does not exceed the final expression we recovered there, squared and multiplied by $\bar{r}^{-1}$, i.e. $CB^2\bar{r}^3\hbar^{-\frac{2}{3}}L_*^2$.

Plugging values of $\hbar$ and θ we arrive to expression (26.5.34) in Proposition 26.5.13(ii) below.

(iii) Due to Chapter 18 the contribution of α_j element to the semiclassical error in T-term does not exceed $CB\ell_*\zeta_*$ as $j=3,2$. Note that $\zeta = G^{\frac{1}{2}}\gamma_0^2\gamma_1^{\frac{3}{2}}\gamma_2\gamma_3^{\frac{1}{2}}$ and $\zeta = G^{\frac{1}{2}}\gamma_0^2\gamma_1^{\frac{3}{2}}\gamma_1$ for $j=3,2$. Here we took $\theta=\alpha=1$ thus covering the whole zone $\mathcal{Y}$.

Then the contribution of α_2-element does not exceed $CBG^{\frac{1}{2}}\bar{r}\gamma_0^3\gamma_1^{\frac{5}{2}}\gamma_2^2$. Further, the contribution of α_1-element does not exceed $CBG^{\frac{1}{2}}\bar{r}\gamma_0^3\gamma_1^{\frac{5}{2}}\int\gamma_2^{-1}\,dx$[32)], resulting in $CBG^{\frac{1}{2}}\bar{r}\gamma_0^3\gamma_1^{\frac{5}{2}}$ in virtue of the same observation (26.5.29).

Further, the contribution of α_0-element does not exceed $CBG^{\frac{1}{2}}\bar{r}\gamma_0^3\int\gamma_1^{-\frac{1}{2}}$ resulting in $CBG^{\frac{1}{2}}\bar{r}\gamma_0^3$ in virtue of the same observation (26.5.30).

Finally, the total contribution of $\mathcal{Y}$ does not exceed $CBG^{\frac{1}{2}}\bar{r} = CB^2\bar{r}^3 = \max(B^{\frac{5}{4}}, Z^{\frac{3}{5}}B^{\frac{4}{5}})$.

Therefore we arrive to

Proposition 26.5.13. *In the framework of Proposition 26.5.13 there exists potential W_ε such that*

(i) Contributions of $\mathcal{Y}^*$ to both semiclassical and approximation errors for N*-term do not exceed*

$$(Z-N)_+^{\frac{1}{4}} L \times (B^{\frac{19}{48}};\ Z^{\frac{7}{20}} B^{\frac{2}{15}}), \tag{26.5.33}$$

where here and below we list different values for $(Z-N)_+^{\frac{4}{3}} \le B \le Z^{\frac{4}{3}}$ and for $Z^{\frac{4}{3}} \le B \le Z^3$.

(ii) Contributions of $\mathcal{Y}^* \times \mathcal{Y}^*$ to both semiclassical and approximation D*-terms do not exceed*

$$(B^{\frac{25}{24}};\ Z^{\frac{1}{2}} B^{\frac{2}{3}}). \tag{26.5.34}$$

(iii) Contributions of $\mathcal{Y}^*$ to both semiclassical and approximation errors for T*-term do not exceed*

$$(B^{\frac{5}{4}};\ Z^{\frac{3}{5}} B^{\frac{4}{5}}). \tag{26.5.35}$$

Case $B \le (Z-N)_+^{\frac{4}{3}}$

Now let us consider the case $B \le (Z-N)_+^{\frac{4}{3}}$. In this case the *boundary strip*

$$\mathcal{Y} := \{x\colon |W(x)+\nu| \le \epsilon|\nu|\} \tag{26.5.36}$$

consists of two subzones

$$\mathcal{Y}_1 := \{x\colon \epsilon B \le |W(x)+\nu| \le \epsilon|\nu|\} \tag{26.5.37}$$

and

$$\mathcal{Y}^* := \{x\colon |W(x)+\nu| \le \epsilon B\}. \tag{26.5.38}$$

Applying arguments of Section 26.4 (more precisely, analysis in zones $\mathcal{X}_1$, $\mathcal{X}_1$ extended and $\mathcal{X}_2$) one can prove easily that

Proposition 26.5.14. *Let $B \le (Z-N)_+^{\frac{4}{3}}$. Then*

(i) Contributions of $\mathcal{Y}_1$ into semiclassical and approximation errors in N*-term do not exceed $C|\nu|\bar{r}^2 \asymp C(Z-N)_+^{\frac{2}{3}}$.*

(ii) Contributions of $\mathcal{Y}_1 \times \mathcal{Y}_1$ *into semiclassical and approximation* D*-terms do not exceed* $C|\nu|^2\bar{r}^3 \asymp C(Z-N)_+^{\frac{5}{3}}$.

(iii) Contribution of $\mathcal{Y}_1$ *into semiclassical and approximation errors in* T*-term do not exceed* $C|\nu|^{\frac{3}{2}}\bar{r} \asymp C(Z-N)_+^{\frac{5}{3}}$.

Proof. We leave easy details to the reader. □

On the other hand, applying arguments of the previous Subsubsection *26.5.3.1. Case* $B \ge (Z-N)_+^{\frac{4}{3}}$ with $\theta = 1$, $\hbar = |\nu|^{-\frac{1}{2}}\bar{r}^{-1} \asymp (Z-N)_+^{-\frac{1}{3}}$ one can prove easily the following

Proposition 26.5.15. *Let* $B \le (Z-N)_+^{\frac{4}{3}}$. *Then*

(i) Contributions of $\mathcal{Y}_2$ *into semiclassical and approximation errors in* N*-term do not exceed* $C(Z-N)_+^{-\frac{5}{9}}B$.

(ii) Contributions of $\mathcal{Y}_2 \times \mathcal{Y}_2$ *into semiclassical and approximation* D*-terms do not exceed* $C(Z-N)_+^{-\frac{7}{9}}B^2$.

(iii) Contribution of $\mathcal{Y}_2$ *into semiclassical and approximation errors in* T*-term do not exceed* $C(Z-N)_+^{\frac{5}{3}}$.

Proof. We leave easy details to the reader.

26.5.4 Summary

Adding contributions of all other zones we arrive to

Proposition 26.5.16. *Let* $M \ge 2$. *Then for the constructed potential* W

(i) Total semiclassical and approximation errors in N*-term do not exceed*

$$C\begin{cases} CZ^{\frac{2}{3}} + (Z-N)_+^{-\frac{5}{9}}B & \text{if } B \le (Z-N)_+^{\frac{4}{3}},\\ Z^{\frac{2}{3}} + B^{\frac{1}{2}}L + (Z-N)_+^{\frac{1}{4}}B^{\frac{19}{48}}L_* & \text{if } (Z-N)_+^{\frac{4}{3}} \le B \le Z^{\frac{4}{3}},\\ Z^{\frac{2}{5}}B^{\frac{1}{5}}L + (Z-N)_+^{\frac{1}{4}}Z^{\frac{7}{20}}B^{\frac{2}{15}}L_* & \text{if } Z^{\frac{4}{3}} \le B \le Z^3 \end{cases} \tag{26.5.39}$$

where $L_* = (1 + |\log\theta|)$ *with* $\theta = |\nu|G^{-1} = (Z-N)_+ \cdot \max(B^{-\frac{3}{4}}, Z^{-1})$ *and* $L = (1 + |\log BZ^3|)$.

(ii) Both semiclassical and approximation D*-terms do not exceed*

$$C\begin{cases} Z^{\frac{5}{3}} + (Z-N)_+^{-\frac{7}{9}}B^2 & \textit{if } B\le (Z-N)_+^{\frac{4}{3}},\\ Z^{\frac{5}{3}} + B^{\frac{5}{4}}L^2 + (Z-N)_+^{\frac{1}{2}}B^{\frac{25}{24}}L_*^2 & \textit{if } (Z-N)_+^{\frac{4}{3}}\le B\le Z^{\frac{4}{3}},\\ Z^{\frac{3}{5}}B^{\frac{4}{5}}L^2 + (Z-N)_+^{\frac{1}{2}}Z^{\frac{1}{2}}B^{\frac{2}{3}}L_*^2 & \textit{if } Z^{\frac{4}{3}}\le B\le Z^3.\end{cases} \tag{26.5.40}$$

(iii) Total approximation error in T*-term does not exceed*

$$CQ := C\max\bigl(Z^{\frac{5}{3}},\, Z^{\frac{3}{5}}B^{\frac{4}{5}}\bigr) = C\begin{cases} Z^{\frac{5}{3}} & \textit{if } B\le Z^{\frac{4}{3}},\\ Z^{\frac{3}{5}}B^{\frac{4}{5}} & \textit{if } Z^{\frac{4}{3}}\le B\le Z^3.\end{cases} \tag{26.5.41}$$

(iv) Total semiclassical error in T*-term does not exceed*

$$CQ + CZ^{\frac{4}{3}}B^{\frac{1}{3}} + CZ^{\frac{3}{2}}a^{-\frac{1}{2}} \tag{26.5.42}$$

provided $a\ge Z^{-1}$*; for* $a\le Z^{-1}$ *the last term should be replaced by* CZ^2*.*

Also we arrive to

Proposition 26.5.17. *Let* $M\ge 2$*,* $B\le Z$ *and* $a\ge Z^{-\frac{1}{3}}$*. Then for the constructed potential* W

(i) Total semiclassical and approximation errors in N*-term do not exceed* $CZ^{\frac{2}{3}}\bigl((BZ^{-1})^{\delta} + (aZ^{\frac{1}{3}})^{-\delta} + Z^{-\delta}\bigr)$*.*

(ii) Both semiclassical and approximation D*-terms and semiclassical and approximation errors in* T*-term do not exceed* $CZ^{\frac{5}{3}}\bigl((BZ^{-1})^{\delta}+(aZ^{\frac{1}{3}})^{-\delta}+Z^{-\delta}\bigr)$*.*

26.6 Ground State Energy

26.6.1 Lower Estimates

Now the lower estimates for the ground state energy E_N are already proven: in virtue of the analysis given in Subsection 25.2.1 we know that

$$\mathsf{E}_N \ge \Phi_*(W) + \Bigl(\operatorname{Tr}(H_{A,W}-\nu)^- + \int P_B(W+\nu)\,dx\Bigr) - \nu N \tag{26.6.1}$$

for *arbitrary* potential W and $\nu \le 0$; picking Thomas-Fermi potential $W = W_B^{\mathsf{TF}}$ and chemical potential ν, we arrive to estimate (26.6.2) below with $W = W_B^{\mathsf{TF}}$ and $Q = 0$.

However we use slightly different potential W and arrive to estimate (26.6.2) below where CQ, defined by (26.5.42), estimates an approximation error; replacing T-term by its semiclassical approximation and applying Proposition 26.5.16(iii) and 26.5.17(ii), we arrive to estimates (26.6.3)–(26.6.6) below:

Proposition 26.6.1. *Let $B \le Z^3$. Then*

(i) The following estimate holds with an approximate potential W we constructed:

$$E^{\mathsf{TF}} \ge \mathcal{E}^{\mathsf{TF}} + \Bigl(\operatorname{Tr}((H_{A,W} - \nu)^-) + \int P_B(W+\nu)\,dx\Bigr) - CQ \tag{26.6.2}$$

with Q defined by (26.5.41)*; further, for $W = W_B^{\mathsf{TF}}$ this estimate holds with $Q = 0$.*

(ii) The following estimates hold for $M = 1$ and $M \ge 2$ respectively

$$E^{\mathsf{TF}} \ge \mathcal{E}^{\mathsf{TF}} + \mathsf{Scott} - CQ - CZ^{\frac{4}{3}}B^{\frac{1}{3}} \tag{26.6.3}$$

and

$$E^{\mathsf{TF}} \ge \mathcal{E}^{\mathsf{TF}} + \mathsf{Scott} - CQ - CZ^{\frac{4}{3}}B^{\frac{1}{3}} - CZ^{\frac{3}{2}}a^{-\frac{1}{2}} \tag{26.6.4}$$

provided $a \ge Z^{-1}$[34] *and $B \le Z^2$; on the other hand, if $a \le Z^{-1}$, we can skip* Scott *and replace the last term in (26.4.2) by CZ^2.*

(iii) As $B \le Z$ the following estimates hold for $M = 1$ and $M \ge 2$, $a \ge Z^{-\frac{1}{3}}$ respectively

$$E^{\mathsf{TF}} \ge \mathcal{E}^{\mathsf{TF}} + \mathsf{Scott} + \mathsf{Dirac} + \mathsf{Schwinger} - CZ^{\frac{5}{3}}\bigl(Z^{-\delta} + (BZ^{-1})^{\delta}\bigr) \tag{26.6.5}$$

and

$$E^{\mathsf{TF}} \ge \mathcal{E}^{\mathsf{TF}} + \mathsf{Scott} + \mathsf{Dirac} + \mathsf{Schwinger} - CZ^{\frac{5}{3}}\bigl(Z^{-\delta} + (BZ^{-1})^{\delta} + (aZ^{\frac{1}{3}})^{-\delta}\bigr). \tag{26.6.6}$$

[34] Recall that a is the minimal distance between nuclei.

26.6.2 Upper Estimate: General Scheme

On the other hand, the upper estimate is more demanding. Recall that, according to Subsection 25.2.2, for the upper estimate in addition to the trace we need to estimate also $|\lambda_N - \nu|$ where $\lambda_N < 0$ is N-th eigenvalue of $H_{A,W}$ and $\lambda_N = 0$ if $H_{A,W}$ has less than N negative eigenvalues, and the product

$$|\lambda_N - \nu| \cdot |\mathsf{N}(H_{A,W}) - N| \tag{26.6.7}$$

and also three D-terms: two of them are semiclassical:

$$\mathsf{D}\Big(e(x,x,\lambda) - P'_B(W(x)+\lambda),\, e(x,x,\lambda) - P'_B(W(x)+\lambda)\Big) \tag*{(26.6.8)$_{1,2}$}$$

with $\lambda = \nu$ and $\lambda = \lambda_N$ and also

$$\mathsf{D}\Big(P'_B(W(x)+\lambda_N) - P'_B(W(x)+\nu),\, P'_B(W(x)+\lambda_N) - P'_B(W(x)+\nu)\Big). \tag{26.6.9}$$

For this purpose our tool will be semiclassical estimates for two semiclassical N-terms

$$\int \Big(e(x,x,\lambda) - P'_B(W(x)+\lambda)\Big)\, dx \tag*{(26.6.10)$_{1,2}$}$$

also with $\lambda = \nu$ and $\lambda = \lambda_N$ and also estimate from below for the third N-term

$$|\int \Big(P'_B(W(x)+\lambda_N) - P'_B(W(x)+\nu)\Big)\, dx|. \tag{26.6.11}$$

26.6.3 Upper Estimate as $M = 1$

Estimate for $|\lambda_N - \nu|$

We start from the easier case $M = 1$. Exactly as in Subsection 25.2.2 we have two cases: in the first case $|\nu|$ is small enough so we construct W^{TF} with $\nu = 0$ and estimate $|\lambda_N|$, and in the second case we prove that $\lambda_N \asymp \nu$ and estimate $|\lambda_N - \nu| \le \epsilon|\nu|$.

Proposition 26.6.2. *Let $M = 1$, $B \le Z^3$.*

(i) Assume first that

$$(Z-N)_+ \le K := C_0 \max\bigl(Z^{\frac{2}{3}},\, Z^{\frac{2}{5}}B^{\frac{1}{5}}\bigr) \tag{26.6.12}$$

and let us construct W *as if* $\nu=0$ *i.e.* $N=Z$. *Then*

$$|\lambda_N| \le C_1 \max\bigl(Z^{\frac{8}{9}},\, B^{\frac{2}{3}}\bigr). \tag{26.6.13}$$

(ii) Assume now that

$$(Z-N)_+ \ge K = C_0 \max\bigl(Z^{\frac{2}{3}},\, Z^{\frac{2}{5}}B^{\frac{1}{5}}\bigr) \tag{26.6.14}$$

with sufficiently large C_0. *Then* $\lambda_N \asymp \nu$ *and*

$$|\lambda_N - \nu| \le C_1 \max\bigl(Z^{\frac{2}{3}},\, B^{\frac{1}{2}}\bigr)|\nu|^{\frac{1}{4}}. \tag{26.6.15}$$

Proof. (i) In the framework of Statement (i) assume first that $B \ge (Z-N)_+^{\frac{4}{3}}$. One can see easily that then

(26.6.16) Expression (26.6.11) is

$$\asymp B|\lambda_N|^{\frac{1}{2}} \times \underbrace{\Bigl(\frac{|\lambda_N|}{G}\Bigr)^{\frac{1}{4}}\bar{r}^3} \asymp |\lambda_N|^{\frac{3}{4}} \min\bigl(1,\, B^{-\frac{3}{10}}Z^{\frac{2}{5}}\bigr)$$

where $(|\lambda_N|/G)^{\frac{1}{4}}\bar{r}$ is a width of the zone where $0 < W \le -\lambda_N$ and the selected factor is the volume of this zone. Indeed, $W \asymp (\bar{r}-|x|)_+^4\bar{r}^{-4}G$ for $|x| \asymp \bar{r}$.

However this expression (26.6.11) should be less than $C\max\bigl(Z^{\frac{2}{3}},\, Z^{\frac{2}{5}}B^{\frac{1}{5}}\bigr)$ which is exactly an error estimate in the semiclassical expression for N. Thus

$$|\lambda_N|^{\frac{3}{4}} \min\bigl(1,\, Z^{\frac{2}{5}}B^{-\frac{3}{10}}\bigr) \le C\max\bigl(Z^{\frac{2}{3}},\, Z^{\frac{2}{5}}B^{\frac{1}{5}}\bigr) \tag{26.6.17}$$

where everywhere the first and the second cases are as $B \le Z^{\frac{4}{3}}$ and $Z^{\frac{4}{3}} \le B \le Z^3$ respectively. The last inequality is equivalent to (26.6.13).

On the other hand, if $B \le (Z-N)_+^{\frac{4}{3}}$, inequality (26.6.17) is replaced by $|\lambda_N|^{\frac{3}{4}} \le CZ^{\frac{2}{3}}$ which coincides with (26.6.17) with B reset to $(Z-N)_+^{\frac{4}{3}}$ and also with the same inequality derived for $B=0$ in Subsection 25.4.2; therefore (26.6.13) holds in this case as well.

(ii) One can prove easily that

(26.6.18) If condition (26.6.14) is fulfilled, and expression (26.6.11) does not exceed the semiclassical error estimate $C_0 \max(Z^{\frac{2}{3}}, Z^{\frac{2}{5}} B^{\frac{1}{5}})$, then $\lambda_N \asymp \nu$ and, furthermore, expression (26.6.11) is

$$\asymp B|\lambda_N - \nu| \int P''_B(W+\nu)\,dx \asymp B|\lambda_N - \nu| \int (W+\nu)_+^{-\frac{1}{2}}\,dx, \tag{26.6.19}$$

which for $B \ge (Z-N)_+^{\frac{4}{3}}$ is

$$\asymp B\bar{r}^3 |\lambda_N - \nu| \cdot |\nu|^{-\frac{1}{2}} \Bigl(\frac{|\nu|}{G}\Bigr)^{\frac{1}{4}} \asymp |\lambda_N - \nu| \cdot |\nu|^{-\frac{1}{4}} \min\bigl(1,\ B^{-\frac{3}{10}} Z^{\frac{2}{5}}\bigr) \tag{26.6.20}$$

and this should be less than $C \max\bigl(Z^{\frac{2}{3}},\ Z^{\frac{2}{5}} B^{\frac{1}{5}}\bigr)$, and this implies (26.6.15).

On the other hand, if $B \le (Z-N)_+^{\frac{4}{3}}$, then the right-hand expression of (26.6.19) is $\asymp |\lambda_N - \nu| \bar{r} \asymp |\lambda_N - \nu| (Z-N)_+^{-\frac{1}{3}}$ and this should be less than $CZ^{\frac{2}{3}}$, and this implies (26.6.15) in this case as well. □

Proposition 26.6.2 immediately implies

Corollary 26.6.3. *In the frameworks of Proposition 26.6.2(i), (ii),*

$$|\lambda_N - \nu| \cdot \mathsf{N}([\lambda_N, \nu]) \le CQ, \tag{26.6.21}$$

where $\mathsf{N}(\lambda_N, \nu)$ *is the number of (non-zero) eigenvalues on interval* $[\lambda_N, \nu]$ *or* $[\nu, \lambda_N]$ [35]*.*

Estimate for D-Terms

Proposition 26.6.4. *In the frameworks of Proposition 26.6.2(i),(ii) expressions*

$$\mathsf{D}\bigl(e(x,x,\lambda) - P'_B(W+\lambda),\ e(x,x,\lambda) - P'_B(W+\lambda)\bigr) \tag{26.6.22}$$

with $\lambda = \nu$ [35] *and with* $\lambda = \lambda_N$ *and*

$$\mathsf{D}\bigl(P'_B(W+\nu) - P'_B(W+\lambda),\ P'_B(W+\nu) - P'_B(W+\lambda_N)\bigr) \tag{26.6.23}$$

with $\lambda = \lambda_N$ *do not exceed* $C \max(Z^{\frac{5}{3}}, Z^{\frac{3}{5}} B^{\frac{4}{5}})$*.*

[35] Recall, that the frameworks of Proposition 26.6.2(i) we pick up $\nu = 0$.

Proof. Recall that we already derived in Section 26.3 this estimate for D-term (26.6.22) with $\lambda = \nu$. Further, the same estimate for this term with $\lambda = \lambda_N$ can be proven exactly in the same way; we leave easy details to the reader.

Furthermore, one can derive the same estimate for D-term (26.6.23) using Proposition 26.6.2; again we leave easy details to the reader. □

Remark 26.6.5. Let $B \le Z$. Then in (26.6.12)–(26.6.15) and therefore also in (26.6.19) and in Proposition 26.6.4 one can replace C_0 and C by $C_0\varepsilon$ and $C\varepsilon$ respectively with the small parameter ε: $\max\bigl(Z^{-\delta}, (BZ^{-1})^{\delta}\bigr) \le \varepsilon \le 1$.

Summary

Then following the scheme of Subsection 25.4.4 we arrive to upper estimates in Theorem 26.6.6 below (lower estimates have been proven in Proposition 26.6.1). Furthermore, based on estimates (26.6.2) and (26.6.24) and the fact, that the left-hand term in (26.6.28) should fit into the "gap" between them (see Section 25.2), we also arrive to Theorem 26.6.7 below:

Theorem 26.6.6. *Let $M = 1$, $B \le Z^3$. Then*

(i) The following estimate holds:

$$E^{\mathsf{TF}} \le \mathcal{E}^{\mathsf{TF}} + \Bigl(\operatorname{Tr}((H_{A,W} - \nu)^-) + \int P_B(W^{\mathsf{TF}}(x) + \nu)\,dx\Bigr) + CQ \tag{26.6.24}$$

with $Q = \max\bigl(Z^{\frac{5}{3}}, Z^{\frac{3}{5}}B^{\frac{4}{5}}\bigr)$.

(ii) The following estimate holds:

$$E^{\mathsf{TF}} \le \mathcal{E}^{\mathsf{TF}} + \mathsf{Scott} + CQ + CZ^{\frac{4}{3}}B^{\frac{1}{3}}. \tag{26.6.25}$$

Here for $Z^2 \le B \le Z^3$ one can skip Scott.

(iii) If $B \le Z$, then

$$E^{\mathsf{TF}} \ge \mathcal{E}^{\mathsf{TF}} + \mathsf{Scott} + \mathsf{Dirac} + \mathsf{Schwinger} + CZ^{\frac{5}{3}}\bigl(Z^{-\delta} + (BZ^{-1})^{\delta}\bigr). \tag{26.6.26}$$

Theorem 26.6.7. *Let $M = 1$, $B \le Z^3$. Then* *(i) The following estimate holds:*

$$\mathsf{D}(\rho_\Psi - \rho_B^{\mathsf{TF}}, \rho_\Psi - \rho_B^{\mathsf{TF}}) \le CQ. \tag{26.6.27}$$

(ii) If $B \le Z$, then

$$\mathsf{D}(\rho_\Psi - \rho_B^{\mathsf{TF}}, \rho_\Psi - \rho_B^{\mathsf{TF}}) \le CZ^{\frac{5}{3}}\bigl(Z^{-\delta} + (BZ^{-1})^{\delta}\bigr). \tag{26.6.28}$$

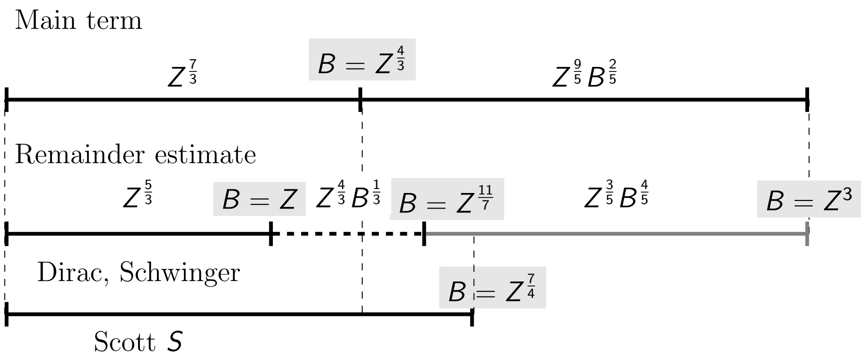

Figure 26.3: This figure illustrates the remainder estimate for E_N. Thresholds $B = Z^\star$ are shown in the yellow boxes.

26.6.4 Upper Estimate as $M \ge 2$

Estimate for $|\lambda_N - \nu|$

Again we need to consider two cases: *almost neutral molecules* (systems) when $(Z-N)_+ \le C_0 K$ with K slightly redefined below and we can set $\nu = 0$ in the definition of Thomas-Fermi potential and establish estimate for $|\lambda_N|$ (and for optimal ν we have the same estimate for both $|\nu|$ and λ_N) and *not almost neutral molecules* (systems) when $(Z-N)_+ \ge C_0 K$ and we can prove that $|\lambda_N| \asymp |\nu|$ and estimate $|\lambda_N - \nu|$.

Proposition 26.6.8 [36]**.** *Let $M \ge 1$, $B \le Z^3$ and condition* (26.2.28) *be fulfilled.*

[36] Cf. Proposition 26.6.2.

(i) Assume first that

$$(Z-N)_+ \le K := C_0 \begin{cases} Z^{\frac{2}{3}} + B^{\frac{1}{2}} L & \text{if } B \le Z^{\frac{4}{3}}, \\ Z^{\frac{1}{5}} B^{\frac{4}{15}} L & \text{if } Z^{\frac{4}{3}} \le B \le Z^3 \end{cases} \tag{26.6.29}$$

and let us construct W *as if* $\nu = 0$ *i.e.* $N = Z$. *Then*

$$|\lambda_N| \le C_1 \begin{cases} Z^{\frac{8}{9}} + B^{\frac{2}{3}} L^{\frac{4}{3}} & \text{if } B \le Z^{\frac{4}{3}}, \\ Z^{\frac{1}{5}} B^{\frac{4}{15}} L^{\frac{4}{3}} & \text{if } Z^{\frac{4}{3}} \le B \le Z^3; \end{cases} \tag{26.6.30}$$

recall that $L = |\log BZ^{-3}|$.

(ii) Assume now that

$$(Z-N)_+ \ge K \tag{26.6.31}$$

with sufficiently large C_0 *in the definition of* K. *Then* $\lambda_N \asymp \nu$ *and moreover*

$$|\lambda_N - \nu| \le C \max\bigl(Z^{\frac{2}{3}}, B^{\frac{1}{2}} L_1\bigr) |\nu|^{\frac{1}{4}}, \tag{26.6.32}$$

where

$$L_1 = \begin{cases} 1 & \text{if } B \le (Z-N)_+^{\frac{4}{3}}, \\ |\log((Z-N)_+/B^{\frac{3}{4}}| & \text{if } (Z-N)_+^{\frac{4}{3}} \le B \le Z^{\frac{4}{3}}, \\ |\log(Z-N)_+/B^{\frac{4}{5}} Z^{\frac{3}{5}}|) & \text{if } Z^{\frac{4}{3}} \le B \le Z^3. \end{cases} \tag{26.6.33}$$

(iii) For $M = 1$ *one can take* $L = L_1 = 1$.

Proof. We will apply arguments slightly more sophisticated than the obvious ones, used in the proof of Proposition 26.6.2. These better arguments will allow us to derive slightly better estimates for $|\lambda_N - \nu|$ as $(Z-N)_+ \ge CK$, and for threshold K itself.

Recall that estimates for $|\lambda_N - \nu|$ are derived by comparison of expression (26.6.11) and the semiclassical errors for the number of eigenvalues below $\lambda = \nu$ and $\lambda = \lambda_N$: expression (26.6.11) should be less than the sum of these semiclassical errors.

Consider contribution of each ball

$$B(x, \ell(x)) \subset \mathcal{Y} = \{x\colon \min_m |x - \mathsf{y}_m| \ge \epsilon \bar{r}\} \tag{26.6.34}$$

to semiclassical errors as $\lambda = \nu$ and $\lambda = \lambda_N$ and compare it with its contribution to (26.6.11):

(a) Each ball contributes no more than $CB\ell^2$ to the first error (with $\lambda=\nu$) where due to our choice $\zeta\ell\ge 1$.

(b) Further, each ball with $\zeta\ge C_1|\lambda_N-\nu|^{\frac12}$ contributes no more than $CB\ell^2$. On the other hand, each ball with $\zeta\le C_1|\lambda_N-\nu|^{\frac12}$ contributes no more than $CB\ell^{3-\sigma}|\lambda_N-\nu|^{\sigma/2}$ to the second error (with $\lambda=\lambda_N$); here $\sigma=\frac13$ is due to rescaling.

(c) Meanwhile, each ball with $\zeta\ge C_1|\lambda_N-\nu|^{\frac12}$ contributes no less than $\epsilon_0 B|\lambda_N-\nu|\zeta^{-1}\ell^3$, and each ball with $\zeta\ge C_1|\lambda_N-\nu|^{\frac12}$ contributes no less than $\epsilon_0|\lambda_N-\nu|^{\frac12}\ell^3$ to expression (26.6.11) and it is larger than the contributions of this ball to each of semiclassical errors (multiplied by C) as long as

$$\zeta^2\ge|\lambda_N-\nu|\ge C_2\zeta\ell^{-1},\qquad |\lambda_N-\nu|\ge C_2\ell^{-2}. \tag{26.6.35$_{1,2}$}$$

Obviously in Statements (i), (ii) we can assume that

(26.6.36) Inequalities (26.6.30) and (26.6.32) respectively (with C replaced by arbitrarily large C_3) are violated.

(i)(a) Assume first that $(Z-N)_+^{\frac43}\le B\le Z^3$. Then in the framework of assumption $\zeta=B^2\ell^4$ with minimal $\ell=B^{-\frac13}$ and therefore $(26.6.35)_{1,2}$ are fulfilled for $\ell\le C_2B^{-1}|\lambda_N|$. Therefore we need to account for the semiclassical errors contributed by an inner shell (not exceeding $C\max(Z^{\frac23},B^{\frac12})$) and by zone $\mathcal{Y}\cap\{\ell\ge C_2B^{-1}|\lambda_N|\}$; there $\zeta\ge C_1|\lambda_N|^{\frac12}$ and therefore its contribution does not exceed $CB\int\ell(x)^{-1}\,dx$ with integral over this zone and it does not exceed $CB\bar{r}^2L$.

So, these truncated semiclassical errors do not exceed $C\max(Z^{\frac23},B\bar{r}^2L)$. Meanwhile, expression (26.6.11) is no less than $CB^{\frac12}\bar{r}^2|\lambda_N|^{\frac34}$. Therefore comparing these two expressions as $B\le Z^{\frac43}$ and as $Z^{\frac43}\le B\le Z^3$ we arrive to (26.6.30).

(b) Consider the remaining case $B\le(Z-N)_+^{\frac43}$. Semiclassical arguments remain valid while estimate of (26.6.11) from below by $\epsilon_0|\lambda_N|^{\frac34}$ also could be proven easily.

(ii)(a) Again, assume first that $(Z-N)_+^{\frac43}\le B\le Z^3$. Again, in the calculation of the truncated semiclassical errors we integrate over zone

$\{\ell \geq C_2 B^{-1}|\lambda_N - \nu|\}$ where $\zeta \geq C_1|\lambda_N|^{\frac{1}{2}}$ and therefore its contribution does not exceed $CB\int \ell(x)^{-1}\,dx$ with integral over this zone and it does not exceed $CB\bar{r}^2 L_1$ [37].

Again, expression (26.6.21) is larger than the expressions afterwards and comparing with the semiclassical error estimate we arrive to (26.6.32).

(b) Consider the remaining case $B \leq (Z-N)_+^{\frac{4}{3}}$. Semiclassical arguments remain valid while estimate of (26.6.11) from below by $\epsilon_0|\lambda_N - \nu|\cdot|\lambda_N|^{-\frac{1}{4}}$ also could be proven easily.

(iii) Recall that for $M = 1$ the semiclassical error estimate hold with $L = L_1 = 1$. □

Then we arrive immediately to

Corollary 26.6.9. *In the framework of Proposition 26.6.8* $|\lambda_N - \nu|\cdot \mathsf{N}([\lambda_N, \nu])$ *does not exceed expression* (26.5.40).

Estimate for D-Terms for Almost Neutral Systems

We need to estimate the semiclassical error D-term (26.6.22) with $\lambda = \lambda_N$ because for $\lambda = \nu$ we already estimated it, and also we need to estimate another D-term (26.6.23). We start from the latter one. Recall that under assumption (26.6.29) we take $\nu = 0$. The trivial estimate is based on

$$|P'_B(W) - P'_B(W+\lambda)| \leq CW^{\frac{1}{2}}|\lambda| + CBW^{-\frac{1}{4}}|\lambda|^{\frac{3}{4}}, \tag{26.6.37}$$

leading to

$$J \leq C\mathsf{D}(W^{\frac{1}{2}},\, W^{\frac{1}{2}})|\lambda|^2 + CB^2|\lambda|^{\frac{3}{2}}\mathsf{D}(W^{-\frac{1}{4}}\theta,\, W^{-\frac{1}{4}}\theta) \tag{26.6.38}$$

where here and below J is expression (26.6.23), θ is a characteristic function of the domain $\{x\colon \gamma(x) \geq h^{\frac{1}{3}}\}$ and we can ignore the contribution of the zone $\{x\colon \gamma(x) \leq h^{\frac{1}{3}}\}$. Really, the contribution of this zone does not exceed a semiclassical error estimate $R := C\max(Z^{\frac{5}{3}},\, Z^{\frac{3}{5}}B^{\frac{4}{5}}L^2)$.

Note that even without assumption (26.6.29)

$$\mathsf{D}(W^{\frac{1}{2}},\, W^{\frac{1}{2}}) \asymp (B^{-\frac{1}{4}};\, B^{-\frac{8}{5}}Z^{\frac{9}{5}}) \qquad \text{for } B \leq Z^{\frac{4}{3}},\, Z^{\frac{4}{3}} \leq B \leq Z^3 \tag{26.6.39}$$

[37] In Statement (i) this leads only to insignificant improvement.

respectively and (26.6.30) implies that the first term in the right-hand expression of (26.6.38) is much less than R.

Meanwhile, under assumption (26.6.29)

$$\mathsf{D}(W^{-\frac{1}{4}}\theta, W^{-\frac{1}{4}}\theta) \asymp B^{-1}\mathsf{D}(\ell^{-1}\theta, \ell^{-1}\theta) \asymp B^{-1}\bar{r}^3\mathsf{D}(\gamma^{-1}\theta, \gamma^{-1}\theta) \tag{26.6.40}$$

where in the right-hand expression D and γ, θ are in the scale $x \mapsto x\bar{r}^{-1}$ and then $\mathsf{D}(\gamma^{-1}\theta, \gamma^{-1}\theta) \asymp L^2$ so the second term in (26.6.38) does not exceed $CB\bar{r}^3|\lambda_N|^{\frac{3}{2}}L^2$ which due to (26.6.30) does not exceed

$$R := C\max\bigl(Z^{\frac{5}{3}},\ Z^{\frac{3}{5}}B^{\frac{4}{5}}L^4\bigr). \tag{26.6.41}$$

Consider now term (26.6.22) with $\lambda = \lambda_N$. Let us consider zones $\Omega_1 := \{x\colon |\lambda - \nu| \lesssim \zeta\ell^{-1}\}$ and $\Omega_2 := \{x\colon |\lambda - \nu| \gtrsim \zeta\ell^{-1}\}$.

Note that the contribution to the term in question of each pair of balls contained in $\Omega_1 \times \Omega_1$ does not exceed estimate for the same term with $\lambda = \nu$; really, after rescaling $x \mapsto x/\ell$ and $\tau \mapsto \tau/\zeta^2$ we conclude that the difference between energy levels does not exceed local semiclassical parameter $C/(\zeta\ell)$.

Therefore the total contribution of $\Omega_1 \times \Omega_1$ to this term does not exceed $C\max\bigl(Z^{\frac{5}{3}},\ Z^{\frac{3}{5}}B^{\frac{4}{5}}L^2\bigr)$.

On the other hand, the contribution to the term in question of each pair of balls contained in $\Omega_2 \times \Omega_2$ does not exceed its contribution to (26.6.25) and therefore the total contribution of $\Omega_2 \times \Omega_2$ to this term does not exceed expression (26.6.41). Thus, term (26.6.22) with $\lambda = \lambda_N$ does not exceed (26.6.41).

Therefore we arrive immediately to

Theorem 26.6.10. *Let $M \ge 2$, $B \le Z^3$ and condition* (26.2.28) *be fulfilled. Then under assumption* (26.6.29)

(i) The following estimate holds:

$$E^{\mathsf{TF}} \le \mathcal{E}^{\mathsf{TF}} + \Bigl(\operatorname{Tr}((H_{A,W} - \nu)^-) + \int P_B(W^{\mathsf{TF}} + \nu)\,dx\Bigr) + C\max\bigl(Z^{\frac{5}{3}},\ Z^{\frac{3}{5}}B^{\frac{4}{5}}L^4\bigr). \tag{26.6.42}$$

(ii) If $a \ge Z^{-1}$ then the following estimate holds:

$$E^{\mathsf{TF}} \le \mathcal{E}^{\mathsf{TF}} + \mathsf{Scott} + C\max\bigl(Z^{\frac{5}{3}},\ Z^{\frac{3}{5}}B^{\frac{4}{5}}L^4\bigr) + CZ^{\frac{4}{3}}B^{\frac{1}{3}} + Ca^{-\frac{1}{2}}Z^{\frac{3}{2}}; \tag{26.6.43}$$

if $a \le Z^{-1}$ one should replace the last term in the right-hand expression by CZ^2 and skip Scott.

(iii) If $B \le Z$ *and* $a \ge Z^{-\frac{1}{3}}$

$$E^{\mathsf{TF}} \le \mathcal{E}^{\mathsf{TF}} + \mathsf{Scott} + \mathsf{Dirac} + \mathsf{Schwinger} + CZ^{\frac{5}{3}}\bigl(Z^{-\delta} + (BZ^{-1})^{\delta} + (aZ^{\frac{1}{3}})^{-\delta}\bigr). \tag{26.6.44}$$

Here proof of Statement (iii) is due to the same arguments as in the case $B=0$. Combining with the estimate from below we also conclude that

Theorem 26.6.11. *(i) In the framework of Theorem 26.6.10 the following estimate holds:*

$$\mathsf{D}\bigl(\rho_\Psi - \rho^{\mathsf{TF}},\, \rho_\Psi - \rho^{\mathsf{TF}}\bigr) \le C\max\bigl(Z^{\frac{5}{3}};\, Z^{\frac{3}{5}}B^{\frac{4}{5}}L^4\bigr). \tag{26.6.45}$$

(ii) In the framework of Theorem 26.6.10(iii) the following estimate holds:

$$\mathsf{D}\bigl(\rho_\Psi - \rho^{\mathsf{TF}},\, \rho_\Psi - \rho^{\mathsf{TF}}\bigr) \le CZ^{\frac{5}{3}}\bigl(Z^{-\delta} + (BZ^{-1})^{\delta} + (aZ^{\frac{1}{3}})^{-\delta}\bigr). \tag{26.6.46}$$

Estimate for D-Terms for Positively Charged Systems

Let assumption (26.6.31) be fulfilled. Let $W = W_\nu$ and $\ell = \ell_\nu$ be a potential and a scaling function (used to derive semiclassical remainder estimates) for this $\nu < 0$ (and $N < Z$) while W_0 and ℓ_0 be a potential and a scaling function for $\nu = 0$ (and $N = Z$).

Let us start from rather trivial arguments. Note that

$$|P'_B(W+\lambda) - P'_B(W+\nu)| \le CW^{\frac{1}{2}}|\lambda-\nu|\theta_1 + CB|\lambda-\nu|^{\frac{1}{2}}\theta_2, \tag{26.6.47}$$

where θ_1 and θ_2 are characteristic functions of $\mathcal{Y}_1 = \{x\colon W(x)+\nu \ge C_0|\nu|\}$ and $\mathcal{Y}_2 = \{x\colon 0 < W(x)+\nu \le C_0|\nu|\}$ respectively. Let

$$J_k \coloneqq \mathsf{D}\bigl([P'_B(W+\lambda_N) - P'_B(W+\nu)]\theta_k,\, [P'_B(W+\lambda_N) - P'_B(W+\nu)]\theta_k\bigr).$$

Then in virtue of (26.6.47)

$$J_1 \le C\mathsf{D}(W^{\frac{1}{2}}\theta_1, W^{\frac{1}{2}}\theta_1)|\lambda_N - \nu|^2.$$

Note that[38)]

$$\mathsf{D}(W^{\frac{1}{2}}\theta_1,\, W^{\frac{1}{2}}\theta_1) \asymp \bigl((Z-N)_+^{-\frac{1}{3}};\, B^{-\frac{1}{4}};\, Z^{\frac{9}{5}}B^{-\frac{8}{5}}\bigr).$$

Then, using inequality (26.6.32) one can prove easily that $J_1 \le CZ^{\frac{5}{3}}$.

However estimate for a contribution of zone $\mathcal{Y}_2$ is much worse:

$$J_2 \le CB^2\mathsf{D}(\theta_2,\theta_2)|\lambda_N-\nu| \le CB^2\bar{r}^3(|\nu|/B^2)^{\frac{1}{2}}L_1^2|\lambda_N-\nu|, \tag{26.6.48}$$

where for $B \le (Z-N)_+^{\frac{1}{3}}$ we should replace $(|\nu|/B^2)^{\frac{1}{2}}L_1^2$ by $\bar{r}^2$. Then, using (26.6.32), we conclude that for $(Z-N)_+^{\frac{4}{3}} \lesssim B \lesssim Z^3$

$$J_2 \le CB\bar{r}^3|\nu|^{\frac{3}{4}}L_1^2\max(Z^{\frac{2}{3}},B^{\frac{1}{2}}) \asymp CB(Z-N)_+^{\frac{3}{4}}\bar{r}^{\frac{9}{4}}\max(Z^{\frac{2}{3}},B^{\frac{1}{2}}L_1)L_1^2,$$

and therefore we arrive to the last two cases below; the first case is proven similarly:

$$J_2 \le C\begin{cases}(Z-N)_+^{-\frac{4}{3}}Z^{\frac{2}{3}}B^2,\\ (Z-N)_+^{\frac{3}{4}}B^{\frac{7}{16}}\max(Z^{\frac{2}{3}},B^{\frac{1}{2}}L_1)L_1^2,\\ (Z-N)_+^{\frac{3}{4}}Z^{\frac{9}{20}}B^{\frac{3}{5}}L_1^3\end{cases} \tag{26.6.49}$$

in our three cases.

This is really shabby estimate. To improve it let us observe that

(26.6.50) If estimate $|\lambda_N-\nu| \le C\max(B^{\frac{2}{3}},(Z-N)_+^{\frac{8}{9}})$ holds, then J_2 does not exceed (26.5.40)

and therefore we can assume that

$$|\lambda_N-\nu| \ge C\max((Z-N)_+^{\frac{8}{9}};\ B^{\frac{2}{3}}). \tag{26.6.51}$$

Let us estimate the truncated semiclassical error[39].

Proposition 26.6.12. *(i) Let* $(Z-N)_+^{\frac{4}{3}} \le B \le Z^3$ *and*

$$C_0B^{\frac{2}{3}} \le |\lambda_N-\nu| \le C_1B^{\frac{1}{2}}|\nu|^{\frac{1}{4}}. \tag{26.6.52}$$

Then the truncated semiclassical error in N*-term does not exceed*

$$F := CZ^{\frac{2}{3}} + CB\bar{r}^2(|\nu|/B^2)^{\frac{1}{4}}L\times(B^{-1}|\lambda_N-\nu|)^{-1}. \tag{26.6.53}$$

[38] In our three cases $B \le (Z-N)_+^{\frac{4}{3}}$, $(Z-N)_+^{\frac{4}{3}} \le B \le Z^{\frac{4}{3}}$, and $Z^{\frac{4}{3}} \le B \le Z^3$ respectively.

[39] I.e. contribution to such error of the zone, where it exceeds the contribution to the principal part.

(ii) Let $(Z-N)_+^{\frac{4}{3}} \le B \le Z^3$ *and*

$$C_1 B^{\frac{1}{2}}|\nu|^{\frac{1}{4}} \le |\lambda_N - \nu| \le C_1 B^{\frac{1}{2}}|\nu|^{\frac{1}{4}} L. \tag{26.6.54}$$

Then the truncated semiclassical error does not exceed

$$F := CZ^{\frac{2}{3}} + CB\bar{r}^2 L. \tag{26.6.55}$$

(iii) Let $B \le (Z-N)_+^{\frac{4}{3}}$ *and*

$$(Z-N)_+^{\frac{8}{9}} \le |\lambda_N - \nu| \le C_1 (Z-N)_+. \tag{26.6.56}$$

Then the truncated semiclassical error does not exceed

$$F := CZ^{\frac{2}{3}} + C(Z-N)_+^{\frac{5}{3}} |\lambda_N - \nu|^{-1}. \tag{26.6.57}$$

(iv) Let $B \le (Z-N)_+^{\frac{4}{3}}$ *and*

$$C_0 (Z-N)_+ \le |\lambda_N - \nu| \le C_1 Z^{\frac{2}{3}} (Z-N)_+^{\frac{1}{3}}. \tag{26.6.58}$$

Then the truncated semiclassical error does not exceed $F := CZ^{\frac{2}{3}}$.

Proof. The easy proof, which uses arguments of the proof of Proposition 26.6.8, is left to the reader. □

Proposition 26.6.13. *In the framework of Proposition 26.6.12(i)–(iv) term* (26.6.25) *does not exceed*

$$CF^{\frac{5}{3}} (B|\lambda_N - \nu|^{\frac{1}{2}})^{\frac{1}{3}} + \text{(26.5.40)}$$

with F *defined in the corresponding cases in Proposition 26.6.12.*

Proof. Using Proposition 26.6.8 one can prove easily that

(26.6.59) Contribution of $\{x\colon \ell(x) := \min_m |x - \mathsf{y}_m| \le \epsilon \bar{r}\}$ to (26.6.25) does not exceed $CZ^{\frac{5}{3}}$.

Now we need to estimate the excess of expression (26.6.25) over semi-classical D-term (with $\lambda=\nu$), which has been estimated by (26.5.40). To do so we need to estimate

$$\mathsf{D}\bigl([P_B(W+\nu)-P_B(W+\lambda)]\theta,\,[P_B(W+\nu)-P_B(W+\lambda)]\theta\bigr) \tag{26.6.60}$$

which is the contribution of the domain $\Omega':=\{x\colon \ell(x)\le CB^{-1}|\lambda-\nu|\}$ where θ is the characteristic function of Ω'. Recall that in the complimentary domain $|P_B(W+\nu)-P_B(W+\lambda)|\le C\ell^{-1}$. Let us consider

$$\mathsf{D}\bigl([P_B(W+\nu)-P_B(W+\lambda)]\theta_0,\,[P_B(W+\nu)-P_B(W+\lambda)]\theta_0\bigr) \tag{26.6.61}$$

and

$$\mathsf{D}\bigl([P_B(W+\nu)-P_B(W+\lambda)]\theta_t,\,[P_B(W+\nu)-P_B(W+\lambda)]\theta_{t'}\bigr), \tag{26.6.62}$$

where θ_0 is a characteristic function of

$$\Omega'_0:=\{x\colon \ell(x)\le t_0:=(|\lambda_N-\nu|B^{-2})^{\frac{1}{4}}\}$$

and θ_t is a characteristic function of $\Omega'_t:=\{x\colon t\le\ell(x)\le 2t\}$ with $t\ge t'\ge t_0$.

Observe that, when calculating expression (26.6.11), the contribution of Ω'_0 is $\asymp B|\lambda_N-\nu|^{\frac{1}{2}}\operatorname{mes}(\Omega'_0)$, and therefore due to Proposition 26.6.12

$$\operatorname{mes}(\Omega'_0)\le CF\bigl(B|\lambda_N-\nu|^{\frac{1}{2}}\bigr)^{-1}, \tag{26.6.63}$$

while term (26.6.61) is

$$\asymp B^2|\lambda_N-\nu|\mathsf{D}(\theta_0,\theta_0)\le CB^2|\lambda_N-\nu|\bigl(\operatorname{mes}(\Omega_0)\bigr)^{\frac{5}{3}}\le CF^{\frac{5}{3}}\bigl(B|\lambda_N-\nu|^{\frac{1}{2}}\bigr)^{\frac{1}{3}},$$

where the middle inequality

$$\mathsf{D}(\chi_G,\chi_G)\le C\bigl(\operatorname{mes}(G)\bigr)^{\frac{5}{3}} \tag{26.6.64}$$

is well known[40] and the last one is due to (26.6.63); χ_G denotes characteristic function of G.

Similarly, when calculating expression (26.6.11), one can see easily that the contribution of Ω'_t is $\asymp B|\lambda_N-\nu|(B^2t^4)^{-1}\operatorname{mes}(\Omega'_t)$ and therefore

$$\operatorname{mes}(\Omega'_t)\le CF|\lambda_N-\nu|^{-1}t^2, \tag{26.6.65}$$

[40] Really, among uniform solids of equal mass and density the ball has the least potential energy; then $C=\frac{1}{5}(12\pi)^{\frac{1}{3}}$.

while term (26.6.62) is $\asymp |\lambda_N-\nu|^2 t^{-2}t'^{-2}\mathsf{D}(\theta_t,\theta_{t'})$, which does not exceed

$$C|\lambda_N-\nu|^2 t^{-2}t'^{-2}\operatorname{mes}(\Omega_t)\operatorname{mes}(\Omega_{t'})\bigl[\max\bigl(\operatorname{mes}(\Omega_t),\ \operatorname{mes}(\Omega_{t'})\bigr)\bigr]^{-\frac{1}{3}} \tag{26.6.66}$$

due to inequality

$$\mathsf{D}(\chi_G,\chi_{G'})\le C\operatorname{mes}(G)\operatorname{mes}(G')\bigl[\max\bigl(\operatorname{mes}(G),\ \operatorname{mes}(G')\bigr)\bigr]^{-\frac{1}{3}}, \tag{26.6.67}$$

which trivially follows from the obvious inequality $\mathsf{D}(\chi_G,\delta_z)\le C(\operatorname{mes}(G))^{\frac{2}{3}}$, where $\delta_z(x)=\delta(x-z)$.

Due to (26.6.65) expression (26.6.66) does not exceed $CF^{\frac{5}{3}}t^{-\frac{2}{3}}$; recall that $t\ge t'$. Since summation with respect to $t\ge t'$ and then with respect to $t'\ge t_0$ returns $CF^{\frac{5}{3}}t_0^{-\frac{2}{3}}$, we conclude that term (26.6.61) with θ_0 replaced by θ'' (the characteristic function of $\{x\colon \ell(x)\ge t_0\}$) also does not exceed $CF^{\frac{5}{3}}(B|\lambda_N-\nu|^{\frac{1}{2}})^{\frac{1}{3}}$. □

So, we have now two estimates for an excess of expression (26.6.25) over (26.5.40): one estimate is

$$CF^{\frac{5}{3}}(B|\lambda_N-\nu|^{\frac{1}{2}})^{\frac{1}{3}} \tag{26.6.68}$$

with $F=F(|\lambda_N-\nu|)$ derived in Proposition 26.6.12 and another one is due to (26.6.48). Let us consider the best of them. Note that estimate (26.6.68) consists of two terms each due to the corresponding term in the definition of F. The second term in the framework of Proposition 26.6.12(i) is

$$C\bigl(B^{\frac{3}{2}}\bar{r}^2|\nu|^{\frac{1}{4}}L|\lambda_N-\nu|^{-1}\bigr)^{\frac{5}{3}}\bigl(B|\lambda_N-\nu|^{\frac{1}{2}}\bigr)^{\frac{1}{3}}\asymp B^{\frac{17}{6}}\bar{r}^{\frac{10}{3}}|\nu|^{\frac{5}{12}}L^{\frac{5}{3}}|\lambda_N-\nu|^{-\frac{3}{2}}.$$

Then, taking minimum of this expression and $CB\bar{r}^3|\nu|^{\frac{1}{2}}L^2|\lambda_N-\nu|$, we see that this minimum does not exceed

$$C\bigl(B^{\frac{17}{6}}\bar{r}^{\frac{10}{3}}|\nu|^{\frac{5}{12}}L^{\frac{5}{3}}\bigr)^{\frac{2}{5}}\bigl(B\bar{r}^3|\nu|^{\frac{1}{2}}L^2\bigr)^{\frac{3}{5}}\asymp CB^{\frac{5}{3}}\bar{r}^{\frac{8}{3}}(Z-N)_+^{\frac{7}{15}}L^{\frac{28}{15}}\asymp\\
C\begin{cases}(Z-N)_+^{\frac{7}{15}}BL^{\frac{28}{15}} & \text{if } (Z-N)_+^{\frac{4}{3}}\le B\le Z^{\frac{4}{3}},\\ (Z-N)_+^{\frac{7}{15}}Z^{\frac{8}{15}}B^{\frac{3}{5}}L^{\frac{28}{15}} & \text{if } Z^{\frac{4}{3}}\le B\le Z^3,\end{cases}$$

which is achieved for $|\lambda_N-\nu|\asymp B^{\frac{11}{15}}\bar{r}^{\frac{2}{15}}|\nu|^{-\frac{1}{30}}L^{-\frac{2}{15}}$. One can see easily that this expression does not exceed (26.5.40).

Therefore in the framework of Proposition 26.6.12(i)(ii) we can select $F=(Z^{\frac{2}{3}}+B\bar{r}^2L)$ according to (26.6.55), arriving to

$$C(Z^{\frac{2}{3}}+B\bar{r}^2L)^{\frac{5}{3}}B^{\frac{1}{3}}|\lambda_N-\nu|^{\frac{1}{6}}\le C(Z^{\frac{2}{3}}+B\bar{r}^2L)^{\frac{5}{3}}B^{\frac{1}{3}}(Z^{\frac{2}{3}}+B^{\frac{1}{2}}L_1)^{\frac{1}{6}}|\nu|^{\frac{1}{24}},$$

which we can rewrite (slightly increasing powers of logarithms) as two last cases in expression

$$C\begin{cases}(Z-N)_+^{\frac{1}{18}}Z^{\frac{11}{9}}B^{\frac{1}{3}} & \text{if } B\le (Z-N)_+^{\frac{4}{3}},\\ (Z-N)_+^{\frac{1}{24}}(Z^{\frac{11}{9}}+B^{\frac{11}{12}}L^4)B^{\frac{11}{32}} & \text{if } (Z-N)_+^{\frac{4}{3}}\le B\le Z^{\frac{4}{3}},\\ (Z-N)_+^{\frac{1}{24}}Z^{\frac{79}{120}}B^{\frac{23}{30}} & \text{if } Z^{\frac{4}{3}}\le B\le Z^3.\end{cases}\tag{26.6.69}$$

In the framework of Proposition 26.6.12(iii) one should replace $(\nu/B^2)^{\frac{1}{4}}$ by $\bar{r}$ and L by 1, so $B^{\frac{3}{2}}\bar{r}^2|\nu|^{\frac{1}{4}}L|\lambda_N-\nu|^{-1}\mapsto B^2\bar{r}^3|\lambda_N-\nu|^{-1}$; further, one should preserve $B|\lambda_N-\nu|^{\frac{1}{2}}$ and therefore the second term becomes

$$\bigl(B^2\bar{r}^3|\lambda_N-\nu|^{-1}\bigr)^{\frac{5}{3}}\bigl(B|\lambda_N-\nu|^{\frac{1}{2}}\bigr)^{\frac{1}{3}}\asymp B^{\frac{11}{3}}\bar{r}^5|\lambda_N-\nu|^{-\frac{3}{2}}$$

and taking minimum of it and (26.6.48) we again get a term lesser than (26.5.40).

Meanwhile, the first term becomes $Z^{\frac{10}{9}}B^{\frac{1}{3}}|\lambda_N-\nu|^{\frac{1}{6}}\le (Z-N)_+^{\frac{1}{18}}Z^{\frac{11}{9}}B^{\frac{1}{3}}$ occupying the first line in (26.6.69).

Therefore we have proven

Proposition 26.6.14. *If $M\ge 2$, $B\le Z^3$ all three* D*-terms do not exceed* (26.5.40) + (26.6.69)*.*

Summary

Therefore all error terms in the upper estimate do not exceed (26.5.40) and we arrive to

Theorem 26.6.15. *Let $M\ge 2$, $B\le Z^3$. Then*

(i) The following estimate holds:

$$E^{\mathsf{TF}}\le \mathcal{E}^{\mathsf{TF}}+\Bigl(\operatorname{Tr}((H_{A,W}-\nu)^-)+\int P_B(W^{\mathsf{TF}}+\nu)\,dx\Bigr)+ \\ (26.5.40)+(26.6.69).\tag{26.6.70}$$

(ii) The following estimate holds for $\mathsf{a} \geq Z^{-1}$*:*

$$E^{\mathsf{TF}} \leq \mathcal{E}^{\mathsf{TF}} + \underbrace{\mathsf{Scott} + CZ^{\frac{4}{3}}B^{\frac{1}{3}} + \mathsf{a}^{-\frac{1}{2}}Z^{\frac{3}{2}}} + (26.5.40) + (26.6.69); \tag{26.6.71}$$

for $\mathsf{a} \leq Z^{-1}$ *one should replace selected terms by* CZ^2*.*

(iii) If $B \leq Z$ *and* $\mathsf{a} \geq Z^{-\frac{1}{3}}$

$$E^{\mathsf{TF}} \geq \mathcal{E}^{\mathsf{TF}} + \mathsf{Scott} + \mathsf{Dirac} + \mathsf{Schwinger} + CZ^{\frac{5}{3}}\bigl(Z^{-\delta} + (BZ^{-1})^{\delta} + (\mathsf{a}Z^{\frac{1}{3}})^{-\delta}\bigr). \tag{26.6.72}$$

We also arrtive to

Theorem 26.6.16. *(i) In the framework of Theorem 26.6.15(i) the following estimate holds:*

$$\mathsf{D}\bigl(\rho_\psi - \rho^{\mathsf{TF}}, \rho_\psi - \rho^{\mathsf{TF}}\bigr) \leq (26.5.40) + (26.6.69). \tag{26.6.73}$$

(ii) In the framework of Theorem 26.6.15(iii) (albeit without assumption $\mathsf{a} \geq Z^{-\frac{1}{3}}$*) the following estimate holds:*

$$\mathsf{D}\bigl(\rho_\psi - \rho^{\mathsf{TF}}, \rho_\psi - \rho^{\mathsf{TF}}\bigr) \leq CQ \coloneqq CZ^{\frac{5}{3}}\bigl(Z^{-\delta} + (BZ^{-1})^{\delta}\bigr). \tag{26.6.74}$$

Remark 26.6.17. In virtue of Remark 26.3.7 we can replace term $CZ^{\frac{4}{3}}B^{\frac{1}{3}}$ to $o(Z^{\frac{4}{3}}B^{\frac{1}{3}})$. This is also true in the case of the better estimates $M = 1$.

We leave to the reader the following easy problem:

Problem 26.6.18. Investigate conditions to $(Z - N)_+$ so that terms (26.5.40) and (26.6.69) do not spoil the upper estimate for E_N or $\mathsf{D}(\rho_\Psi - \rho_B^{\mathsf{TF}},\ \rho_\Psi - \rho_B^{\mathsf{TF}})$.

26.7 Negatively Charged Systems

In this section we following Section 25.5 consider the case $N \geq Z$ and provide upper estimates for the excessive negative charge $(N - Z)$ if $\mathsf{I}_N > 0$ and for the ionization energy I_N.

26.7.1 Estimates of the Correlation Function

First of all we provide some estimates which will be used for both negatively and positively charged systems. Let us consider the ground-state function $\Psi(x_1,\varsigma_1;\ldots;x_N,\varsigma_N)$ and the corresponding density $\rho_\Psi(x)$. Again the crucial role play estimates[41)]

$$\mathsf{D}\bigl(\rho_\psi-\rho^{\mathsf{TF}},\rho_\psi-\rho^{\mathsf{TF}}\bigr)\le \bar{Q} \tag{26.7.1}$$

where $\bar{Q}\ge Q$ is just the right-hand expression of the corresponding estimate; as $B\le Z$ we can slightly decrease $\bar{Q}=Q$.

Recall that the same estimate holds also for difference between upper and lower bounds for E_N (with $\mathsf{Tr}((H_W-\nu)^-)+\nu N$ not replaced by its semiclassical approximation).

Remark 26.7.1. All arguments and conclusions of Subsection 25.5.1 up to but excluding estimate (25.5.31) are not related to the Schrödinger operator and remain true.

So we need to calculate both the semiclassical errors and the principal parts. Note that *all semiclassical errors for W_ε do not exceed those obtained for W we selected*. Consider approximations errors in the principal part, namely

$$\mathsf{D}\bigl(P'(W_\varepsilon+\nu)-P'(W+\nu),P'(W_\varepsilon+\nu)-P'(W+\nu)\bigr) \tag{26.7.2}$$

and

$$\mathsf{D}(\rho_\varepsilon-\rho,\rho_\varepsilon-\rho) \tag{26.7.3}$$

since we already estimated terms $\mathsf{D}\bigl(P'(W+\nu)-\rho_B^{\mathsf{TF}},P'(W+\nu)-\rho_B^{\mathsf{TF}}\bigr)$ and $\mathsf{D}(\rho-\rho_B^{\mathsf{TF}},\rho-\rho_B^{\mathsf{TF}})$ by $\bar{Q}$.

Note that

$$|W-W_\varepsilon|\le C(1+\ell\varepsilon^{-1})^{-2}\zeta^2 \tag{26.7.4}$$

and

$$|P'(W_\varepsilon+\nu)-P'(W+\nu)|\le C(1+\ell\varepsilon^{-1})^{-2}\zeta^3+C(1+\ell\varepsilon^{-1})^{-1}\zeta B \tag{26.7.5}$$

41) Namely, estimate (26.6.27) of Theorem 26.6.7 if $M=1$, and similar estimates (26.6.45) of Theorem 26.6.11 and (26.6.73) of Theorem 26.6.16 if $M\ge 2$. For $B\le Z$ and $a\ge Z^{-\frac{1}{3}}$, we use estimate (26.6.74) in all cases.

and therefore expression (26.7.2) does not exceed $C\bigl(Z^3\varepsilon^2 + ZB^2\varepsilon^2\bar{r}^2\bigr)$ and it does not exceed $C\max(Z^{\frac{5}{3}}, B^{\frac{4}{5}}Z^{\frac{3}{5}})$ for $\varepsilon=\min(Z^{-\frac{2}{3}}, Z^{\frac{2}{5}}B^{-\frac{4}{5}})$ and this does not exceed $C\bar{Q}$.

Further, consider expression (26.7.3); it is equal to $4\pi|(W_\varepsilon - W, \rho_\varepsilon-\rho)|$ and one can prove easily the same estimate for it.

Furthermore, under this restriction an error in the principal part of asymptotics of $\int e(x,x,\lambda)\,dx$, namely $|\int \bigl(P'(W_\varepsilon+\nu)-P'(W+\nu)\bigr)\,dx|$, does not exceed $C\bigl(Z^{\frac{3}{2}}\varepsilon^{\frac{3}{2}} + Z^{\frac{1}{2}}B\varepsilon\bar{r}^{\frac{3}{2}}\bigr)$, which is less than the semiclassical error. Then $S\le C\bar{Q}$ with S defined by (25.5.22).

So, the following proposition is proven:

Proposition 26.7.2 [42]**.** *If θ,χ are as in Subsection 25.5.2, then estimate* (25.5.33) *holds, namely,*

$$\mathcal{J} = |\int \Bigl(\rho^{(2)}_\Psi(x,y)-\rho(y)\rho_\Psi(x)\Bigr)\theta(x)\chi(x,y)\,dxdy| \le \\ C\sup_x \|\nabla_y\chi_x\|_{\mathscr{L}^2(\mathbb{R}^3)}\Bigl((\bar{Q}+\varepsilon^{-1}N+T)^{\frac{1}{2}}\Theta + P^{\frac{1}{2}}\Theta^{\frac{1}{2}}\Bigr) + C\varepsilon N\|\nabla_y\chi\|_{\mathscr{L}^\infty}\Theta \tag{26.7.6}$$

with $\Theta=\Theta_\Psi$ defined by (25.5.15) *and T,P defined by* (25.5.23), (25.5.25) *and arbitrary $\varepsilon\le\min(Z^{-\frac{2}{3}}, Z^{\frac{2}{5}}b^{-\frac{4}{5}})$.*

Recall that $\rho^{(2)}_\Psi(x,y)$ defined by (25.5.13) is the *quantum correlation function*.

26.7.2 Excessive Negative Charge

Let us select $\theta=\theta_b$ according to (25.5.34):

$$\mathsf{supp}(\theta)\subset\{x\colon \ell(x)\ge b\}. \tag{25.5.34}$$

Note that $\mathsf{H}_N\Psi=\mathsf{E}_N\Psi$ yields identity (25.5.35) and isolating the contribution of j-th electron in j-th term we get inequality (25.5.36):

$$-\mathsf{I}_N\int \rho_\Psi(x)\ell(x)\theta\,dx \ge \\ \sum_j \langle\Psi, \ell(x_j)\theta(x_j)\Bigl(-V(x_j)+\sum_{k:k\ne j}|x_j-x_k|^{-1}\Bigr)\Psi\rangle - \sum_j \|\nabla\bigl(\theta^{\frac{1}{2}}(x_j)\ell(x_j)^{\frac{1}{2}}\bigr)\Psi\|^2 \tag{25.5.36}$$

[42] Cf. Proposition 25.5.1.

due to the non-negativity of operator $\bigl((D_x - A(x))\cdot\boldsymbol{\sigma}\bigr)^2$.

Now let us select b to be able to calculate the magnitude of Θ. Note that inequality (25.5.37) holds. Also (25.5.38) holds as long as

$$Z^{-\frac{1}{3}} \le b \le \epsilon \min\bigl((Z-N)_+^{-\frac{1}{3}}, B^{-\frac{1}{4}}\bigr) \tag{26.7.7}$$

Using inequalities

$$|\nabla(\theta_b(x)^{\frac{1}{2}}\ell^{\frac{1}{2}})| \le cb^{-1}\theta_{(1-\epsilon)b}(x)$$

and

$$\int \rho_\Psi(x)\ell(x)\theta_b(x)\,dx \ge b\Theta_b$$

(i.e. (25.5.43)) we conclude that

$$\begin{aligned} b\mathsf{I}_N\Theta_b \le \int \theta_b(x)V(x)\ell(x)\rho_\Psi(x)\,dx\\ -\int \rho^{(2)}_\Psi(x,y)\ell(x)|x-y|^{-1}\theta_b(x)\,dxdy + Cb^{-1}\Theta_{b(1-\epsilon)} =\\ = \int \theta_b(x)V(x)\ell(x)\rho_\Psi(x)\,dx\\ -\int \rho^{(2)}_\Psi(x,y)\ell(x)|x-y|^{-1}\bigl(1-\theta_b(y)\bigr)\theta_b(x)\,dxdy\\ -\int \rho^{(2)}_\Psi(x,y)\ell(x)|x-y|^{-1}\theta_b(y)\theta_b(x)\,dxdy + Cb^{-1}\Theta_{b(1-\epsilon)} \end{aligned} \tag{26.7.8}$$

(cf. (25.5.44)). Denote by $\mathcal{I}_1$, $\mathcal{I}_2$, and $\mathcal{I}_3$ the first, second and third terms in the right-hand expression of (26.7.8) respectively. Symmetrizing $\mathcal{I}_3$ with respect to x and y

$$\mathcal{I}_3 = -\frac{1}{2}\int \rho^{(2)}_\Psi(x,y)\bigl(\ell(x)+\ell(y)\bigr)|x-y|^{-1}\theta(y)\theta(x)\,dxdy$$

and using inequality $\ell(x)+\ell(y) \ge \min_j(|x-\mathsf{y}_j| + |y-\mathsf{y}_j|) \ge |x-y|$ we conclude that this term does not exceed

$$\begin{aligned} -\frac{1}{2}\int \rho^{(2)}_\Psi(x,y)\theta_b(y)\theta_b(x)\,dxdy =\\ -\frac{1}{2}(N-1)\int \rho_\Psi(x)\theta_b(x)\,dx + \frac{1}{2}\int \rho^{(2)}_\Psi(x,y)\bigl(1-\theta_b(y)\bigr)\theta_b(x)\,dxdy \end{aligned} \tag{26.7.9}$$

(cf. (25.5.45)).

Here the first term is exactly $-\frac{1}{2}(N-1)\Theta_b$; replacing $\rho^{(2)}_\Psi(x,y)$ by $\rho(y)\rho_\Psi(x)$ we get

$$\frac{1}{2}\int \bigl(1-\theta_b(y)\bigr)\rho(y)\,dy \times \Theta_b \tag{26.7.10}$$

with an error

$$\frac{1}{2}\int \bigl(\rho^{(2)}_\Psi(x,y)-\rho(y)\rho_\Psi(x)\bigr)\bigl(1-\theta_b(y)\bigr)\theta_b(x)\,dxdy \tag{26.7.11}$$

(cf. (25.5.46), (25.5.47)). We estimate this expression using Proposition 26.7.2 with $\chi(x,y)=1-\theta_b(y)$. Then $\|\nabla_y\chi_x\|_{\mathscr{L}^2}\asymp b^{\frac{1}{2}}$, $\|\nabla_y\chi\|_{\mathscr{L}^\infty}\asymp b^{-1}$ and $P\asymp b^{-1}\Theta_b$ [43], while $T\lesssim b^{-4}$ as long as $B\le Z^{\frac{4}{3}}$ and $b\le B^{-\frac{1}{4}}$.

To estimate the excessive negative charge we assume that $(N-Z)>0$ with $\mathsf{I}_N>0$. In this case the left-hand expression in (26.7.8) should be positive.

Remark 26.7.3. Recall that in Subsection 25.5.2 we picked $b=Z^{-\frac{5}{21}}$ and it makes sense here as well as long as $b\le\bar{r}=B^{-\frac{1}{4}}$ i.e. as $B\le Z^{\frac{20}{21}}$. However for $B\ge Z^{\frac{20}{21}}$ we just pick up $b=C_0\bar{r}$ and then $T=0$ in our framework.

Estimating (26.7.11) we conclude that

$$\mathcal{I}_3\le -\frac{1}{2}\Bigl(N-1-\int\bigl(1-\theta_b(y)\bigr)\rho(y)\,dy\Bigr)\Theta_b+\mathcal{I}_0 \tag{26.7.12}$$

with

$$\mathcal{I}_0=Cb^{\frac{1}{2}}\Bigl(\mathcal{S}\Theta_b+Nb^{-2}\Bigr)^{\frac{1}{2}}\Theta_b^{\frac{1}{2}}+C\varepsilon Nb^{-1}\Theta_b \tag{26.7.13}$$

(cf. (25.5.48)).

On the other hand,

$$\mathcal{I}_2\le -\int \rho^{(2)}_\Psi(x,y)\ell(x)|x-y|^{-1}\bigl(1-\theta_{b(1-\epsilon)}(y)\bigr)\theta_b(x)\,dxdy \tag{26.7.14}$$

[43] Recall that $P=\int|\nabla\theta^{\frac{1}{2}}|^2\rho_\Psi\,dx$ and $T=\sup_{\mathsf{supp}(\theta)}W$.

and replacing $\rho^{(2)}_\Psi(x,y)$ by $\rho(y)\rho_\Psi(x)$ and estimating an error due to Proposition 26.7.2 again, we get

$$\begin{aligned}(26.7.15)\quad \mathcal{I}_2 \le -\int \rho(y)\rho_\Psi(x)\ell(x)|x-y|^{-1}\bigl(1-\theta_{b(1-\epsilon)}(y)\bigr)\theta_b(x)\,dxdy+\\ Cb^{-\frac{1}{2}}\bigl(\mathcal{S}\Theta_b+Nb^{-2}\bigr)^{\frac{1}{2}}\Theta_b^{\frac{1}{2}}+C\varepsilon Nb^{-1}=\\ -\int (V-W)(x)\ell(x)\theta_b(x)\,dx+\\ \int \rho(y)\rho_\Psi(x)\ell(x)|x-y|^{-1}\theta_{b(1-\epsilon)}(y))\theta_b(x)\,dxdy+\mathcal{I}_0.\end{aligned}$$

So, we picked up

$$(26.7.16)\qquad b = C\min(Z^{-\frac{5}{21}},\bar{r}) = \begin{cases} Z^{-\frac{5}{21}} & \text{if } B\le Z^{\frac{20}{21}},\\ B^{-\frac{1}{4}} & \text{if } Z^{\frac{20}{21}}\le B\le Z^{\frac{4}{3}},\\ B^{-\frac{2}{5}}Z^{\frac{1}{5}} & \text{if } Z^{\frac{4}{3}}\le B\le Z^{3}\end{cases}$$

and

$$(26.7.17)\qquad \varepsilon = \min(Z^{-\frac{2}{3}}, B^{-\frac{4}{5}}Z^{\frac{2}{5}}).$$

Then, preserving all the estimates one can take $W=\rho=0$ at $\mathsf{supp}(\theta_{\frac{b}{2}})$ [44] and then

$$\begin{aligned}(26.7.18)\quad \mathcal{I}_1+\mathcal{I}_2 = \int \theta_b(x)W(x)\ell(x)\rho_\Psi(x)\,dx-\\ \int\Bigl(\rho^{(2)}_\Psi(x,y)-\rho_\Psi(x)\rho(y)\Bigr)\ell(x)|x-y|^{-1}\bigl(1-\theta_b(y)\bigr)\theta_b(x)\,dxdy\le\mathcal{I}_0.\end{aligned}$$

Further, since $\int\bigl(1-\theta_b(y)\bigr)\rho(y)\,dy\le Z$ [45] we get from (26.7.8) and estimate (26.7.12) for $\mathcal{I}_3$ that

$$(26.7.19)\qquad (N-Z)\le Cb^{\frac{1}{2}}\mathcal{S}^{\frac{1}{2}}+C\Theta_b^{-\frac{1}{2}}N^{\frac{1}{2}}b^{-1}+Cb^{-1}\Theta_{b(1-\epsilon)}\Theta_b^{-1}$$

because then $\varepsilon N^{\frac{1}{2}}b^{-1}$ does not exceed $Cb^{\frac{1}{2}}\bar{Q}^{\frac{1}{2}}$.

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[44] For $B\ge Z^{\frac{20}{21}}$ this is fulfilled automatically.

[45] Actually for $B\ge Z^{\frac{20}{21}}$ this is an equality.

Let us assume that estimate (26.7.20) below does not hold. Then $\Theta_b = N - \int (1-\theta_b(y))\rho_\Psi(y)\,dy$ and due to Theorem 26.6.16

$$|\Theta_b - N - Z| \le Cb^{\frac{1}{2}}\bar{Q}^{\frac{1}{2}} \le \frac{1}{2}(N-Z)$$

and the same is true for $\Theta_{b(1-\epsilon)}$. Then (26.7.19) yields (26.7.20). So, (26.7.20) has been proven.

Thus we proved the following theorem:

Theorem 26.7.4. *Let condition* (26.2.28) *be fulfilled. In the fixed nuclei model let* $\mathsf{I}_N > 0$.

(i) Then

$$(N-Z)_+ \le C\begin{cases} Z^{\frac{5}{7}} & \text{if } B\le Z^{\frac{20}{21}},\\ Z^{\frac{5}{6}}B^{-\frac{1}{8}} + B^{\frac{1}{2}}L & \text{if } Z^{\frac{20}{21}}\le B\le Z^{\frac{4}{3}}L\\ Z^{\frac{2}{5}}B^{\frac{1}{5}}L & \text{if } Z^{\frac{4}{3}}\le B\le Z^{3}\end{cases}\tag{26.7.20}$$

where $L = |\log(Z^{-3}B)|$.

(ii) For $M=1$ *the same estimate holds with* $L=1$*:*

$$(N-Z)_+ \le C\begin{cases} Z^{\frac{5}{7}} & \text{if } B\le Z^{\frac{20}{21}},\\ Z^{\frac{5}{6}}B^{-\frac{1}{8}} & \text{if } Z^{\frac{20}{21}}\le B\le Z^{\frac{4}{3}}L\\ Z^{\frac{2}{5}}B^{\frac{1}{5}} & \text{if } Z^{\frac{4}{3}}\le B\le Z^{3}.\end{cases}\tag{26.7.21}$$

Furthermore, for $B\le Z$ one can use a slightly sharper estimate for $\bar{Q}$:

Theorem 26.7.5. *Let condition* (26.2.28) *be fulfilled. In the fixed nuclei model let* $\mathsf{I}_N > 0$. *Then for a single atom and for molecule with* $B \le Z$ *and* $a \ge Z^{-\frac{1}{3}+\delta_1}$

$$(N-Z)_+ \le C\begin{cases} Z^{\frac{5}{7}-\delta} & \text{if } B\le Z^{\frac{20}{21}},\\ Z^{\frac{5}{6}-\delta}B^{-\frac{1}{8}+\delta} & \text{if } Z^{\frac{20}{21}}\le B\le Z\end{cases}\tag{26.7.22}$$

Results for a free nuclei model follow from the above results and an estimate of a from below (see Subsubsection *26.8.4.4. Estimate for Excessive Negative Charge and Ionization Energy*).

Theorem 26.7.6. *Let condition* (26.2.28) *be fulfilled. In the free nuclei model let* $\hat{\mathsf{I}}_N > 0$. *Then*

(i) Estimate (26.7.20) *holds.*

(ii) For $B \le Z$ *estimate* (26.7.22) *holds.*

26.7.3 Estimate for Ionization Energy

Finally, let us estimate the ionization energy, assuming that

(26.7.23) $(Z-N)_+$ does not exceed the right-hand expression of (26.7.20)[46].

Few cases are possible:

(i) $B \le Z^{\frac{20}{21}}$ and $(Z-N)_+ \le C_0 Z^{\frac{5}{7}}$. In this case we act exactly as in Subsection 25.5.2: we pick up $b = \epsilon Z^{-\frac{5}{21}}$ with a small enough constant $\epsilon' > 0$; then

$$|\int \theta_b(x)\bigl(\rho_\Psi - \rho\bigr)\,dx| \le Cb^{\frac{1}{2}} Q^{\frac{1}{2}}, \tag{26.7.24}$$

while

$$\int \theta_b(x)\rho\,dx \asymp b^{-3} \tag{26.7.25}$$

and therefore

$$\Theta := \int \theta_b(x)\rho_\Psi\,dx \asymp b^{-3} \tag{26.7.26}$$

and

$$|\int \theta(x)\bigl(\rho_\Psi - \rho\bigr)\,dx| \le \epsilon''\Theta. \tag{26.7.27}$$

Then (26.7.8), (26.7.12), (26.7.15) yield that $\mathsf{I}_N \le CZ^{\frac{20}{21}}$; so estimate (26.7.37) below in this case is recovered.

In all other cases one needs to replace θ_b by a function which is not b-admissible.

(ii) Let $Z^{\frac{20}{21}} \le B \le Z^3$ and $M=1$. Let here $\bar{r}$ be the exact radius of $\mathsf{supp}(\rho)$, $\rho = \rho_B^{\mathsf{TF}}$ and $W = W_B^{\mathsf{TF}}$, which were obtained in the Thomas-Fermi theory with $\nu = 0$. Recall that $\bar{r} \asymp \max(B^{-\frac{1}{4}};\, B^{-\frac{2}{5}} Z^{\frac{1}{5}})$ and $\bar{Q} \asymp \max(Z^{\frac{5}{3}};\, B^{\frac{4}{5}} Z^{\frac{3}{5}})$. Also recall that $W \asymp Gt^4$ and $\rho \asymp BG^{\frac{1}{2}}$ for $r = (1-t)\bar{r}$ with $1-\epsilon \le t \le 1$, where $G := \min(B;\, B^{\frac{2}{5}} Z^{\frac{4}{5}})$.

We take in this case $\bar{r}t$-admissible function θ, equal 0 for $|x - \mathsf{y}| \le \bar{r}(1-t)$ and equal 1 for $|x-\mathsf{y}| \ge \bar{r}(1-\frac{1}{2}t)$.

(26.7.28) In all the above estimates one needs to replace $Cb^{-1}\Theta_{b(1-\epsilon)}$ by $C\bar{r}^{-1}t^{-1}\Theta'$ with Θ' defined by θ' which is also $\bar{r}t$-admissible and equal 1 in $\epsilon\bar{r}t$-vicinity of $\mathsf{supp}(\theta)$.

[46] Or (26.7.21), or (26.7.22) in the framework of the corresponding theorem.

Then (26.7.24)–(26.7.27) are replaced by

$$|\int \theta(x)\bigl(\rho_\Psi-\rho\bigr)\,dx| \le CQ^{\frac{1}{2}}\times \|\nabla\theta\| \asymp Ct^{-\frac{1}{2}}\bar{r}^{\frac{1}{2}}Q^{\frac{1}{2}} \tag{26.7.29}$$

while

$$\int \theta(x)\rho\,dx \asymp BG^{\frac{1}{2}}\bar{r}^3t^3 \tag{26.7.30}$$

and therefore

$$\Theta := \int \theta(x)\rho_\Psi\,dx \asymp BG^{\frac{1}{2}}\bar{r}^3t^3. \tag{26.7.31}$$

Then (26.7.27) holds provided the right-hand expression of (26.7.29) does not exceed the right-hand expression of (26.7.31), multiplied by ϵ:

$$t=t_*:=C_0B^{-\frac{2}{7}}G^{-\frac{1}{7}}\bar{r}^{-\frac{5}{7}}Q^{\frac{1}{7}} = C_1\max(B^{-\frac{1}{4}}Z^{\frac{5}{21}};\ B^{\frac{2}{35}}Z^{-\frac{6}{35}}) \tag{26.7.32}$$

where we picked up the smallest possible value of t. Note that

$$t\asymp 1 \text{ as either } B\asymp Z^{\frac{20}{21}} \text{ or } B\asymp Z^3. \tag{26.7.33}$$

Further, let us estimate from above

$$\begin{aligned}\mathcal{I}' = -\int \Bigl(\rho^{(2)}_\Psi(x,y)-\rho_\Psi(x)\rho(y)\Bigr)\ell(x)|x-y|^{-1}\theta(x)\,dxdy \le\\ -\int \Bigl(\rho^{(2)}_\Psi(x,y)-\rho_\Psi(x)\rho(y)\Bigr)\bigl(1-\omega_\tau(x,y)\bigr)\ell(x)|x-y|^{-1}\theta(x)\,dxdy +\\ \int \rho_\Psi(x)\rho(y)\omega_\tau(x,y)\ell(x)|x-y|^{-1}\theta(x)\,dxdy\end{aligned} \tag{26.7.34}$$

with $\omega=0$ as $|x-y|\ge 2\tau\bar{r}$ and $\omega=1$ as $|x-y|\le\tau\bar{r}$, with $\tau\in(t,1)$.

Then due to Proposition 26.7.2 with $\chi(x,y)=\bigl(1-\omega_\tau(x,y)\bigr)|x-y|^{-1}$ the first term in the right-hand expression does not exceed $C\bar{r}^{\frac{1}{2}}\tau^{-\frac{1}{2}}Q^{\frac{1}{2}}\Theta$ since $\|\nabla_y\chi_x\|_{\mathscr{L}^2(\mathbb{R}^3)}\asymp(\bar{r}\tau)^{-\frac{1}{2}}$ and also one can prove easily that all other terms in $\Bigl((Q+\varepsilon^{-1}N+T)^{\frac{1}{2}}\Theta+P^{\frac{1}{2}}\Theta^{\frac{1}{2}}\Bigr)$ do not exceed $CQ\Theta$.

Meanwhile, the second term in in the right-hand expression of (26.7.34) does not exceed $CBG^{\frac{1}{2}}\tau^2\times\bar{r}^3\tau^2\times\Theta$ because $\rho(y)\le CBG^{\frac{1}{2}}\tau^2$ if $|x-y|\le 2\tau\bar{r}$, $x\in\operatorname{supp}(\theta)$ and therefore $\int\rho(y)\omega_\tau(x,y)\,dy\le CBG^{\frac{1}{2}}\tau^4$.

Minimizing their sum

$$C\Bigl(\bar{r}^{\frac{1}{2}}\tau^{-\frac{1}{2}}Q^{\frac{1}{2}}+BG^{\frac{1}{2}}\bar{r}^{3}\tau^{4}\Bigr)\Theta$$

with respect to $\tau \ge t$ [47], we arrive to estimate

$$\mathcal{I}' \le C\bar{r}^{\frac{7}{9}}Q^{\frac{4}{9}}B^{\frac{1}{9}}G^{\frac{1}{18}}\Theta.$$

Then exactly as in the proof of Theorem 25.5.3 we have inequality

$$\bar{r}\,\mathsf{I}_N \le C(Z-N)_+ + C\bar{r}^{\frac{7}{9}}Q^{\frac{4}{9}}B^{\frac{1}{9}}G^{\frac{1}{18}}, \tag{26.7.35}$$

and therefore for $(Z-N)_+ \le C\bar{r}^{\frac{7}{9}}Q^{\frac{4}{9}}B^{\frac{1}{9}}G^{\frac{1}{18}}$ we arrive to the estimate $\mathsf{I}_N \le C\bar{r}^{-\frac{2}{9}}Q^{\frac{4}{9}}B^{\frac{1}{9}}G^{\frac{1}{18}}$.

Thus we have proven estimate (26.7.37) of Theorem 26.7.7 below, at least as $N \ge Z$. Further, estimate (26.7.39) under the same assumption $N \ge Z$ is due to the fact that for $B \le Z$ one can use $\bar{Q} = Z^{\frac{5}{3}}(B^{\delta}Z^{-\delta}+Z^{-\delta})$ instead of Q.

Theorem 26.7.7. *Let $M=1$.*

(i) Then for $B \le Z^3$ and

$$(Z-N)_+ \le C_0\begin{cases} Z^{\frac{5}{7}} & \textit{if}\ \ B\le Z^{\frac{20}{21}},\\ B^{-\frac{1}{8}}Z^{\frac{5}{6}} & \textit{if}\ \ Z^{\frac{20}{21}}\le B\le Z^{\frac{4}{3}},\\ B^{\frac{1}{5}}Z^{\frac{2}{5}} & \textit{if}\ \ Z^{\frac{4}{3}}\le B\le Z^{3}\end{cases} \tag{26.7.36}$$

the following estimate holds

$$\mathsf{I}_N \le C\begin{cases} Z^{\frac{20}{21}} & \textit{if}\ \ B\le Z^{\frac{20}{21}},\\ B^{\frac{2}{9}}Z^{\frac{20}{27}} & \textit{if}\ \ Z^{\frac{20}{21}}\le B\le Z^{\frac{4}{3}}\\ B^{\frac{26}{45}}Z^{\frac{4}{15}} & \textit{if}\ \ Z^{\frac{4}{3}}\le B\le Z^{3}.\end{cases} \tag{26.7.37}$$

(ii) Furthermore for $B \le Z$ and

$$(Z-N)_+ \le C_0\begin{cases} Z^{\frac{5}{7}-\delta} & \textit{if}\ \ B\le Z^{\frac{20}{21}},\\ B^{-\frac{1}{8}+\delta}Z^{\frac{5}{6}-\delta} & \textit{if}\ \ Z^{\frac{20}{21}}\le B\le Z\end{cases} \tag{26.7.38}$$

[47] One can see easily that minimum is achieved as $\tau \asymp t^{\frac{7}{9}}$.

the following estimate holds

$$\mathsf{I}_N \le C\begin{cases} Z^{\frac{20}{21}-\delta'} & \textit{if}\ \ B\le Z^{\frac{20}{21}},\\ B^{\frac{2}{9}+\delta'}Z^{\frac{20}{27}-\delta'} & \textit{if}\ \ Z^{\frac{20}{21}}\le B\le Z.\end{cases}\tag{26.7.39}$$

Proof in the general settings. To prove estimates (26.7.37) and (26.7.39) in the general settings (i.e. without assumption $N\ge Z$) observe that for $N<Z$

$$\begin{multline}\mathsf{D}(\rho_N^{\mathsf{TF}}-\rho_Z^{\mathsf{TF}},\,\rho_N^{\mathsf{TF}}-\rho_Z^{\mathsf{TF}})\le C(Z-N)^2\bar{r}^{-1}\asymp\\ C\max\bigl((Z-N)^{\frac{7}{3}};\ C(Z-N)^2B^{\frac{1}{4}};\ C(Z-N)^2B^{\frac{2}{5}}Z^{-\frac{1}{5}}\bigr)\end{multline}\tag{26.7.40}$$

(where subscript here denotes the number of electrons rather than the intensity of the magnetic field) because the same estimate holds for $\mathcal{E}_N^{\mathsf{TF}}-\mathcal{E}_Z^{\mathsf{TF}}$:

$$0\le\mathcal{E}_N^{\mathsf{TF}}-\mathcal{E}_Z^{\mathsf{TF}}\le C(Z-N)^2\bar{r}^{-1},\tag{26.7.41}$$

which itself follows from

$$\frac{\partial\mathcal{E}^{\mathsf{TF}}}{\partial N}=\nu\asymp(Z-N)\bar{r}^{-1}.\tag{26.7.42}$$

Therefore to preserve our estimates we need to assume that the right-hand expression of (26.7.40) does not exceed Q; this assumption is equivalent to $(Z-N)_+\le\min(Z^{\frac{5}{7}};\ Z^{\frac{5}{6}}B^{-\frac{1}{8}})$ for $B\le Z^{\frac{4}{3}}$ which is exactly the first and the second cases in (26.7.36) (and these cases in (26.7.38) appear in the same way), and to $(Z-N)_+\le CB^{\frac{1}{5}}Z^{\frac{2}{5}}$ for $Z^{\frac{4}{3}}\le B\le Z^3$, which is exactly the third case in (26.7.40).

Also there is a term $C(Z-N)_+\bar{r}^{-1}$ in the estimate of I_N. However, under assumption (26.7.40) this term does not exceed the right hand expression of (26.7.40) or (26.7.42), in fact coincides with it only in the first case. □

Consider now $M\ge 2$. Assume that $B\ge Z^{\frac{20}{21}}$ since the opposite case has been analyzed already.

Let us pick up $\bar{r}t$-admissible function θ such that $\theta=1$ if $W\le C_0Gt^4$ and $\theta=0$ if $W\ge 2C_0Gt^4$. In this case ($M\ge 2$) we can claim only that $\|\nabla\theta\|\le Ct^{-\frac{1}{2}}\bar{r}^{\frac{1}{2}}|\log t|^{\frac{1}{2}}$ and therefore

$$|\int\theta(x)\bigl(\rho_\Psi-\rho\bigr)\,dx|\le Ct^{-\frac{1}{2}}|\log t|^{\frac{1}{2}}\bar{r}^{\frac{1}{2}}\bar{Q}^{\frac{1}{2}},\tag{26.7.29$'$}$$

while

$$BG^{\frac{1}{2}}\bar{r}^3t^3 \lesssim \int \theta(x)\rho\, dx \lesssim BG^{\frac{1}{2}}|\log t|\bar{r}^3t^3 \tag{26.7.30$'$}$$

and therefore

$$\Theta := \int \theta(x)\rho_\Psi\, dx \gtrsim BG^{\frac{1}{2}}\bar{r}^3t^3 \tag{26.7.31$'$}$$

for

$$t \ge t_* := C_0B^{-\frac{2}{7}}G^{-\frac{1}{7}}\bar{r}^{-\frac{5}{7}}\bar{Q}^{\frac{1}{7}}|\log t|^{\frac{2}{7}}. \tag{26.7.32$'$}$$

Now we need to look more carefully at $\bar{Q}$, especially because while it may contain "rogue" factor L or L^2, it can also be large as $(Z-N)_+$ is large. Fortunately, this is not the case in the current framework:

Proposition 26.7.8. *(i) Under condition* (26.7.46) *below* $\bar{Q}$ *is as in the case* $N=Z$ *i.e.*

$$\bar{Q} = \begin{cases} Z^{\frac{5}{3}} + B^{\frac{5}{4}}L^2 & \textit{if}\ \ B\le Z^{\frac{4}{3}},\\ B^{\frac{4}{5}}Z^{\frac{3}{5}}L^2 & \textit{if}\ \ Z^{\frac{4}{3}}\le B\le Z^3. \end{cases} \tag{26.7.43}$$

(ii) Furthermore, if $B\le Z$ *and* $a\ge Z^{-\frac{1}{3}}$ *under condition* (26.7.48) *below* $\bar{Q}$ *is exactly as in the case* $N=Z$*, i.e.*

$$\bar{Q} = Z^{\frac{5}{3}}\bigl(Z^{-\delta} + (aZ^{\frac{1}{3}})^{-\delta} + (BZ^{-1})^{\delta}\bigr). \tag{26.7.44}$$

Proof. One can either derive it from the existing estimates or just repeat estimates with $\nu=0$ adding $(Z-N)_+^2\bar{r}^{-1}$ to $\bar{Q}$. We leave easy details to the reader.

Therefore all the above arguments could be repeated with this new expression $\bar{Q}$ which also acquires factor $|\log t|$ (due to this factor in the estimate of $\|\nabla\theta\|$ and this factor boils to $L_1^{\frac{1}{2}}$ with

$$L_1 = \begin{cases} |\log BZ^{-\frac{20}{21}}|+1 & Z^{\frac{20}{21}}\le B\le Z^{\frac{4}{3}},\\ |\log BZ^{-3}|+1 & Z^{\frac{4}{3}}\le B\le Z^3. \end{cases} \tag{26.7.45}$$

Therefore we arrive to

Theorem 26.7.9. *Let* $M\ge 2$*. Then* *(i) For*

$$(Z-N)_+ \le C_0 \begin{cases} Z^{\frac{5}{7}} & \textit{if } B\le Z^{\frac{20}{21}},\\ Z^{\frac{5}{6}}B^{-\frac{1}{8}} + B^{\frac{1}{2}}L & \textit{if } Z^{\frac{20}{21}} \le B \le Z^{\frac{4}{3}},\\ B^{\frac{1}{5}}Z^{\frac{2}{5}}L & \textit{if } Z^{\frac{4}{3}} \le B\le Z^3 \end{cases} \tag{26.7.46}$$

the following estimate holds

$$\mathsf{I}_N \le CL_1^{\frac{2}{9}} \begin{cases} Z^{\frac{20}{21}} & \textit{if } B\le Z^{\frac{20}{21}},\\ Z^{\frac{20}{27}}B^{\frac{2}{9}} + B^{\frac{7}{9}}L^{\frac{8}{9}} & \textit{if } Z^{\frac{20}{21}} \le B \le Z^{\frac{4}{3}}\\ Z^{\frac{4}{15}}B^{\frac{26}{45}}L^{\frac{8}{9}} & \textit{if } Z^{\frac{4}{3}} \le B\le Z^3. \end{cases} \tag{26.7.47}$$

(ii) Furthermore, for $B\le Z$, $a\ge Z^{-\frac{1}{3}}$ and

$$(Z-N)_+ \le C_0\varsigma^{\delta} \begin{cases} Z^{\frac{5}{7}} & \textit{if } B\le Z^{\frac{20}{21}},\\ Z^{\frac{5}{6}}B^{-\frac{1}{8}} & \textit{if } Z^{\frac{20}{21}} \le B \le Z, \end{cases} \tag{26.7.48}$$

with

$$\varsigma = Z^{-1} + BZ^{-1} + a^{-1}Z^{\frac{1}{3}} \tag{26.7.49}$$

the following estimate holds

$$\mathsf{I}_N \le CL_1^{\frac{2}{9}}\varsigma^{\delta'} \begin{cases} Z^{\frac{20}{21}} & \textit{if } B\le Z^{\frac{20}{21}},\\ Z^{\frac{20}{27}}B^{\frac{2}{9}} & \textit{if } Z^{\frac{20}{21}} \le B \le Z. \end{cases} \tag{26.7.50}$$

26.8 Positively Charged Systems

Now let us estimate from above and below the ionization energy in the case when $N<Z$ and condition (26.7.36) (if $M=1$) or (26.7.46) (if $M\ge 2$) fails. We also estimate excessive the positive charge in the case of $M\ge 2$ and free nuclei model. We will follow arguments of the corresponding three subsections of Section 25.6.

26.8.1 Upper Estimate for Ionization Energy: $M=1$

Consider first the case of $M=1$. Then for $B=0$ arguments are well-known (see Section 25.6) but we repeat them for $B>0$: we pick up β-admissible function θ such that $\theta = 1$ if $|x - \mathsf{y}_1| \ge \bar{r} - \beta$ and $\theta = 0$ if $|x - \mathsf{y}_1| \le \bar{r} - 2\beta$ where $\bar{r}$ is an exact radius of support of ρ^{TF} (see the very beginning of Subsection 25.6.1) and $\beta \ll \bar{r}$. Recall that

$$\bar{r} \asymp \begin{cases} (Z-N)^{-\frac{1}{3}} & \text{if } B \le Z^{\frac{20}{21}}, \\ \min\bigl((Z-N)^{-\frac{1}{3}}, B^{-\frac{1}{4}}\bigr) & \text{if } Z^{\frac{20}{21}} \le B \le Z^{\frac{4}{3}}, \\ B^{-\frac{2}{5}} Z^{\frac{1}{5}} & \text{if } Z^{\frac{4}{3}} \le B \le Z^3, \end{cases} \tag{26.8.1}$$

where in the first case we used that $Z - N \ge Z^{\frac{5}{7}}$ while in the second case both subcases $(Z-N)^{-\frac{1}{3}} \gtrless B^{-\frac{1}{4}}$ are possible.

We can assume without any loss of the generality that $\mathsf{y}_1 = 0$. Now in the spirit of Subsection 25.6.1 we need to select as we did in Subsection 26.7.3 the smallest β such that

$$\Theta^{\mathsf{TF}} := \int \theta(x)\rho^{\mathsf{TF}}(x)\,dx \ge C\beta^{-\frac{1}{2}}\bar{r}\bar{Q}^{\frac{1}{2}} \tag{26.8.2}$$

implying that

$$\Theta_\Psi := \int \theta(x)\rho_\Psi(x)\,dx \asymp \Theta^{\mathsf{TF}}, \tag{26.8.3}$$

where the right-hand expression of (26.8.2) estimates $|\int \theta(x)(\rho^{\mathsf{TF}} - \rho_\Psi)\,dx|$ (recall that it does not exceed $\|\nabla\theta\| \cdot \mathsf{D}(\rho^{\mathsf{TF}} - \rho_\Psi, \rho^{\mathsf{TF}} - \rho_\Psi)^{\frac{1}{2}}$). Again as in Subsection 25.6.1 $\rho^{\mathsf{TF}} = \rho^{\mathsf{TF}}_N$ is calculated for the actual value of $N < Z$.

Then, following Subsubsection 25.6.1, eventually we arrive to estimate (25.6.8), namely:

$$\begin{aligned} \mathsf{I}_N \int \ell(x)\rho_\Psi(x)\theta(x)\,dx \le \int \theta(x)V(x)\ell(x)\rho_\Psi(x)\,dx \\ - \int \Bigl(\rho^{(2)}_\Psi(x,y) - \rho_\Psi(x)\rho(y)\Bigr)\ell(x)|x-y|^{-1}\theta(x)\,dxdy \\ - \int \rho_\Psi(x)\rho(y)\ell(x)|x-y|^{-1}\theta(x)\,dxdy + C\beta^{-2}\bar{r}\Theta, \end{aligned} \tag{26.8.4}$$

and then estimate from above the second term in the right-hand expression

$$\begin{aligned} - \int \Bigl(\rho^{(2)}_\Psi(x,y) - \rho_\Psi(x)\rho(y)\Bigr)\ell(x)|x-y|^{-1}\theta(x)\,dxdy \le \\ - \int \Bigl(\rho^{(2)}_\Psi(x,y) - \rho_\Psi(x)\rho(y)\Bigr)\bigl(1 - \omega(x,y)\bigr)\ell(x)|x-y|^{-1}\theta(x)\,dxdy \\ + \int \rho_\Psi(x)\rho(y)\omega(x,y)\ell(x)|x-y|^{-1}\theta(x)\,dxdy \end{aligned} \tag{26.8.5}$$

with $\omega=\omega_\gamma$: $\omega=0$ if $|x-y|\ge 2\gamma$ and $\omega=1$ if $|x-y|\le\gamma$, $\gamma\ge\beta$ (see (25.6.9)).

To estimate the first term in the right-hand expression of (26.8.5) one can apply Proposition 25.5.1. In this case $\|\nabla_y\chi\|_{\mathscr{L}^2}\asymp C\bar{r}\gamma^{-\frac{1}{2}}$, $\|\nabla_y\chi\|_{\mathscr{L}^\infty}\asymp\bar{r}\gamma^{-2}$ and plugging $P=\beta^{-2}\Theta$ and $T=|\nu|$, $\varepsilon=Z^{-\frac{2}{3}}$ we conclude that this term does not exceed (25.6.10)

$$C\bar{r}\bigl(\gamma^{-\frac{1}{2}}Q^{\frac{1}{2}}+Z^{\frac{1}{3}}\gamma^{-2}\bigr)\Theta \tag{26.8.6}$$

(if $Q\ge Z^{\frac{5}{3}}$; otherwise here we should reset here $Q:=Z^{\frac{5}{3}}$).

Note that if $0\le\bar{r}-|x|\asymp\beta$

$$W+\nu\asymp\upsilon:=\max\Bigl\{\bigl(\frac{|\nu|\beta}{\bar{r}}\bigr);\ G\bigl(\frac{\beta}{\bar{r}}\bigr)^4\Bigr\}, \tag{26.8.7}$$

with G defined by (26.2.41) and therefore

$$\rho\asymp\max\Bigl\{\bigl(\frac{|\nu|\beta}{\bar{r}}\bigr)^{\frac{3}{2}};\ B\bigl(\frac{|\nu|\beta}{\bar{r}}\bigr)^{\frac{1}{2}};\ BG^{\frac{1}{2}}\bigl(\frac{\beta}{\bar{r}}\bigr)^2\Bigr\} \tag{26.8.8}$$

where the first and the second clauses are forks of the first clause in (26.8.7) since in the second clause automatically $W+\nu\le B$ for $0\le\bar{r}-|x|\lesssim\beta$; therefore

$$\int\rho(x)\theta(x)\,dx\asymp\max\Bigl\{\bigl(\frac{|\nu|\beta}{\bar{r}}\bigr)^{\frac{3}{2}};\ \ B\bigl(\frac{|\nu|\beta}{\bar{r}}\bigr)^{\frac{1}{2}};\ BG^{\frac{1}{2}}\bigl(\frac{\beta}{\bar{r}}\bigr)^2\Bigr\}\beta\bar{r}^2, \tag{26.8.9}$$

and therefore (26.8.2) holds if and only if

$$\max\Bigl\{\bigl(\frac{|\nu|}{\bar{r}}\bigr)^{\frac{3}{2}}\beta^3;\ \ B\bigl(\frac{|\nu|}{\bar{r}}\bigr)^{\frac{1}{2}}\beta^2;\ BG^{\frac{1}{2}}\bigl(\frac{1}{\bar{r}}\bigr)^2\beta^{\frac{7}{2}}\Bigr\}\bar{r}\ge CQ^{\frac{1}{2}}; \tag{26.8.10}$$

then

$$\beta=\min\Bigl\{Q^{\frac{1}{6}}|\nu|^{-\frac{1}{2}}\bar{r}^{\frac{1}{6}};\ B^{-\frac{1}{2}}Q^{\frac{1}{4}}|\nu|^{-\frac{1}{4}}\bar{r}^{-\frac{1}{4}};\ B^{-\frac{2}{7}}G^{-\frac{1}{7}}Q^{\frac{1}{7}}\bar{r}^{\frac{2}{7}}\Bigr\} \tag{26.8.11}$$

and in the corresponding cases

$$\upsilon=\Bigl\{Q^{\frac{1}{6}}|\nu|^{\frac{1}{2}}\bar{r}^{-\frac{5}{6}};\ B^{-\frac{1}{2}}Q^{\frac{1}{4}}|\nu|^{\frac{3}{4}}\bar{r}^{-\frac{5}{4}};\ B^{-\frac{8}{7}}G^{\frac{3}{7}}Q^{\frac{4}{7}}\bar{r}^{-\frac{20}{7}}\Bigr\}. \tag{26.8.12}$$

Observe, however, that for $B\lesssim Q^{\frac{4}{7}}$ and $|\nu|\lesssim Q^{\frac{4}{7}}$ we do not need these arguments; simpler arguments of Subsection 25.5.3 show that in this case $|\mathsf{I}_N|\le CQ^{\frac{4}{7}}$.

On the other hand, for $B \lesssim Q^{\frac{4}{7}}$ but $|\nu| \gtrsim Q^{\frac{4}{7}}$, we pick $\gamma = Q^{\frac{1}{8}}|\nu|^{-\frac{15}{32}}$, like in Subsection 25.6.1, and observe that $|\nu|\bar{r}^{-1}\gamma \gtrsim B$ and therefore we conclude that $\mathsf{I}_N + \nu \le CQ^{\frac{1}{6}}|\nu|^{\frac{17}{24}}$, exactly like in that subsection. Therefore we arrive to

Proposition 26.8.1. *Let* $B \le C_0 Z^{\frac{20}{21}}$. *Then*

(i) If $|\nu| \le C_0 Z^{\frac{20}{21}}$, *then estimate* $\mathsf{I}_N \le CZ^{\frac{20}{21}}$ *holds like in the case* $B = 0$.

(ii) If $|\nu| \ge C_0 Z^{\frac{20}{21}}$, *then estimate* $\mathsf{I}_N + \nu \le CZ^{\frac{5}{18}}|\nu|^{\frac{17}{24}}$ *holds like in the case* $B = 0$.

Therefore in what follows we assume that $B \ge Q^{\frac{4}{7}}$. One can see easily that then $\beta \le \bar{r}$.

Meanwhile, the same arguments imply that the second term in the right-hand expression of (26.8.5) is of magnitude

$$\max\Bigl\{\bigl(\frac{|\nu|\gamma}{\bar{r}}\bigr)^{\frac{3}{2}};\ B\bigl(\frac{|\nu|\gamma}{\bar{r}}\bigr)^{\frac{1}{2}};\ BG^{\frac{1}{2}}\bigl(\frac{\gamma}{\bar{r}}\bigr)^{2}\Bigr\}\gamma^2$$

and we need to minimize

$$\gamma^{-\frac{1}{2}}Q^{\frac{1}{2}} + \max\Bigl\{\bigl(\frac{|\nu|\gamma}{\bar{r}}\bigr)^{\frac{3}{2}},\quad B\bigl(\frac{|\nu|\gamma}{\bar{r}}\bigr)^{\frac{1}{2}};\ BG^{\frac{1}{2}}\bigl(\frac{\gamma}{\bar{r}}\bigr)^{2}\Bigr\}\gamma^2,$$

which is achieved when

$$\gamma^{-\frac{1}{2}}Q^{\frac{1}{2}} \asymp \max\Bigl\{\bigl(\frac{|\nu|\gamma}{\bar{r}}\bigr)^{\frac{3}{2}};\ B\bigl(\frac{|\nu|\gamma}{\bar{r}}\bigr)^{\frac{1}{2}};\ BG^{\frac{1}{2}}\bigl(\frac{\gamma}{\bar{r}}\bigr)^{2}\Bigr\}\gamma^2.$$

Let us compare this equation with equation to β. It is the same albeit with factor $\bar{r}^2$ rather than γ^2. Therefore if $\gamma \ge \bar{r}$ then $\gamma \le \beta \le \bar{r}$ which is a contradiction. Thus $\gamma \le \bar{r}$ but then $\gamma \ge \beta$.

Therefore we conclude that this term does not exceed

$$\varsigma := \max\Bigl\{Q^{\frac{7}{16}}\bigl(\frac{|\nu|}{\bar{r}}\bigr)^{\frac{3}{16}};\ Q^{\frac{5}{12}}B^{\frac{1}{6}}\bigl(\frac{|\nu|}{\bar{r}}\bigr)^{\frac{1}{12}};\ Q^{\frac{4}{9}}B^{\frac{1}{9}}G^{\frac{1}{18}}\bar{r}^{-\frac{2}{9}}\Bigr\}, \tag{26.8.13}$$

and to estimate $\mathsf{I}_N + \nu$ we need just to compute its sum with υ defined by (26.8.12).

Therefore we conclude that

$$\mathsf{I}_N + \nu \le C(\upsilon + \varsigma). \tag{26.8.14}$$

Remark 26.8.2. Observe that

$$\upsilon(Z,B,|\nu|)=Z^{\frac{20}{21}}\upsilon(1,Z^{-\frac{20}{21}}B,|\nu|Z^{-\frac{20}{21}}|\nu|)\quad \text{if}\quad Z^{\frac{20}{21}}\le B\le Z^{\frac{4}{3}} \tag{26.8.15}$$

and

$$\upsilon(Z,BZ^{-3},|\nu|)=Z^{2}\upsilon(1,Z^{-3}B,|\nu|Z^{-2}|\nu|)\quad \text{if}\quad Z^{\frac{4}{3}}\le B\le Z^{3}, \tag{26.8.16}$$

and ς has the same scaling properties.

Therefore we can make all calculations with $Z=1$ and then scale. Leaving easy calculations to the reader, we arrive to

Proposition 26.8.3. *(i) For* $Z^{\frac{20}{21}}\le B\le Z^{\frac{4}{3}}$

$$I_N+\nu\le C\begin{cases} Z^{\frac{5}{18}}|\nu|^{\frac{17}{24}} & \textit{if}\ \ |\nu|\ge Z^{-\frac{20}{51}}B^{\frac{24}{17}},\\ Z^{\frac{5}{12}}B^{-\frac{1}{2}}|\nu|^{\frac{17}{16}} & \textit{if}\ \ B\le|\nu|\le Z^{-\frac{20}{51}}B^{\frac{24}{17}},\\ Z^{\frac{5}{48}}B^{-\frac{3}{16}}|\nu|^{\frac{3}{4}} & \textit{if}\ \ Z^{\frac{5}{12}}B^{\frac{9}{16}}\le|\nu|\le B,\\ Z^{\frac{25}{36}}B^{\frac{3}{16}}|\nu|^{\frac{1}{12}} & \textit{if}\ \ Z^{\frac{5}{9}}B^{\frac{5}{12}}\le|\nu|\le Z^{\frac{5}{9}}B^{\frac{9}{16}},\\ Z^{\frac{20}{27}}B^{\frac{2}{9}} & \textit{if}\ \ |\nu|\le Z^{\frac{5}{9}}B^{\frac{5}{12}}. \end{cases} \tag{26.8.17}$$

(ii) In particular,

$$I_N\le CZ^{\frac{20}{27}}B^{\frac{2}{9}}\qquad \textit{if}\ \ |\nu|\le Z^{\frac{20}{27}}B^{\frac{2}{9}}. \tag{26.8.18}$$

(iii) For $Z^{\frac{4}{3}}\le B\le Z^{3}$

$$I_N+\nu\le C\begin{cases} Z^{\frac{7}{30}}B^{\frac{8}{15}}|\nu|^{\frac{1}{12}} & \textit{if}\ \ |\nu|\ge Z^{\frac{2}{5}}B^{\frac{8}{15}},\\ Z^{\frac{4}{15}}B^{\frac{26}{45}} & \textit{if}\ \ |\nu|\le Z^{\frac{2}{5}}B^{\frac{8}{15}}. \end{cases} \tag{26.8.19}$$

(iv) In particular,

$$I_N\le CZ^{\frac{4}{15}}B^{\frac{26}{45}}\qquad \textit{if}\ \ |\nu|\le Z^{\frac{4}{15}}B^{\frac{26}{45}}. \tag{26.8.20}$$

Remark 26.8.4. Recall that $Q=Z^{\frac{5}{3}}\bigl(B^{\delta}+1\bigr)Z^{-\delta}$ if $B\le Z$; therefore we can add factor $\bigl(B^{\delta'}+1\bigr)Z^{-\delta'}$ in all estimates of Propositions 26.8.1 and 26.8.3.

26.8.2 Lower Estimate for Ionization Energy: $M = 1$

Now let us derive an estimate $\mathsf{I}_N + \nu$ from below. Let $\Psi = \Psi_N(x_1, \dots, x_N)$ be the ground state for N electrons, $\|\Psi\| = 1$; consider an antisymmetric *test function*

$$\tilde{\Psi} = \tilde{\Psi}(x_1, \dots, x_{N+1}) = \Psi(x_1, \dots, x_N)u(x_{n+1}) - \sum_{1\le j\le N} \Psi(x_1, \dots, x_{j-1}, x_{N+1}, x_{j+1}, \dots, x_N)u(x_j) \tag{26.8.21}$$

Then exactly as in Subsection 25.6.2

$$\begin{aligned}
&\mathsf{E}_{N+1}\|\tilde{\Psi}\|^2 \le \langle \mathsf{H}_{N+1}\tilde{\Psi}, \tilde{\Psi}\rangle = N\langle \mathsf{H}_{N+1}\Psi u, \tilde{\Psi}\rangle = \\
&\quad N\langle \mathsf{H}_N\Psi u, \tilde{\Psi}\rangle + N\langle H_{V,x_{N+1}}\Psi u, \tilde{\Psi}\rangle + N\langle \sum_{1\le i\le N} |x_i - x_{N+1}|^{-1}\Psi u, \tilde{\Psi}\rangle = \\
&\quad (\mathsf{E}_N - \nu')\|\tilde{\Psi}\|^2 + N\langle H_{W+\nu',x_{N+1}}\Psi u, \tilde{\Psi}\rangle \\
&\qquad\qquad + N\langle \bigl(\sum_{1\le i\le N} |x_i - x_{N+1}|^{-1} - (V - W)(x_{N+1})\bigr)\Psi u, \tilde{\Psi}\rangle
\end{aligned}$$

and therefore

$$\begin{aligned}
N^{-1}(\mathsf{I}_{N+1} + \nu')\|\tilde{\Psi}\|^2 \ge &-\langle H_{W+\nu',x_{N+1}}\Psi u, \tilde{\Psi}\rangle \\
&- \langle \bigl(\sum_{1\le i\le N} |x_i - x_{N+1}|^{-1} - (V - W)(x_{N+1})\bigr)\Psi u, \tilde{\Psi}\rangle
\end{aligned} \tag{26.8.22}$$

and

$$\begin{aligned}
N^{-1}\|\tilde{\Psi}\|^2 = &\|\Psi\|^2 \cdot \|u\|^2 - \\
&N\int \Psi(x_1, \dots, x_{N-1}, x)\Psi^\dagger(x_1, \dots, x_{N-1}, y)u(y)u^\dagger(x)\,dx_1\cdots dx_{N-1}\,dxdy
\end{aligned} \tag{26.8.23}$$

as in (25.6.14) and (25.6.15) respectively where † means a complex or Hermitian conjugation and $\nu' \ge \nu$ to be chosen later.

Note that every term in the right-hand expression in (26.8.22) is the sum of two terms: one with $\tilde{\Psi}$ replaced by $\Psi(x_1, \dots, x_N)u(x_{N+1})$ and another with $\tilde{\Psi}$ replaced by $-N\Psi(x_1, \dots, x_{N-1}, x_{N+1})u(x_N)$. We call these terms, as in Subsection 25.6.2, *direct* and *indirect* respectively.

Obviously, in the direct and indirect terms u appears as $|u(x)|^2\,dx$ and as $u(x)u^\dagger(y)\,dxdy$ respectively multiplied by some kernels.

Recall that u is an arbitrary function. Let us take $u(x)=\theta^{\frac{1}{2}}(x)\phi_j(x)$ where ϕ_j are orthonormal eigenfunctions of $H_{W+\nu}$ and $\theta(x)$ is β-admissible function which is supported in $\{x\colon -\upsilon\ge W(x)+\nu\ge \frac{2}{3}\nu\}$ and equal 1 in $\{x\colon -2\upsilon\ge W(x)+\nu\ge\frac{1}{2}\nu\}$, satisfying (25.5.11), and υ is related to β as in the previous Section 26.7:

$$\upsilon = C\max(\nu\bar{r}^{-1}\beta;\ G\bar{r}^{-4}\beta^4). \tag{26.8.24}$$

Let us substitute it into (26.8.22), multiply by $\varphi(\lambda_j L^{-1})$ and take the sum with respect to j; then we get the same expressions with $|u(x)|^2\,dx$ and $u(x)u^\dagger(y)\,dxdy$ replaced by $F(x,x)\,dx$ and $F(x,y)\,dxdy$ respectively with

$$F(x,y)=\int \varphi(\lambda L^{-1})\,d_\lambda e(x,y,\lambda). \tag{26.8.25}$$

Here $\varphi(\tau)$ is a fixed $\mathscr{C}^\infty$ non-negative function equal to 1 for $\tau\le\frac{1}{2}$ and equal to 0 for $\tau\ge 1$ and $L=\nu'-\nu=6\upsilon$.

Under described construction and procedures the direct term generated by $N^{-1}\|\tilde{\Psi}\|^2$ is

$$\int \theta(x)\varphi(\lambda L^{-1})\,d_\lambda e(x,x,\lambda)\,dx. \tag{26.8.26}$$

Then, applying semiclassical approximation, we get

$$\Theta_\Psi := \int \varphi(\lambda L^{-1})\,d_\lambda P'_B(W+\nu-\lambda)\,dx. \tag{26.8.27}$$

Consider the remainder estimate. Assume that $M=1$ (case $M\ge 2$ will be considered later). Then since $L=C_1\upsilon$ the remainder does not exceed

$$Ch^s(\mu h+1)\beta^{-2}\bar{r}^2, \tag{26.8.28}$$

where

$$h=1/(\upsilon^{\frac{1}{2}}\beta) \tag{26.8.29}$$

and

$$\mu = B\beta\upsilon^{-\frac{1}{2}}; \tag{26.8.30}$$

one can prove it easily by partition of unity on $\mathsf{supp}(\theta)$ and applying semiclassical asymptotics with effective semiclassical parameter h and magnetic parameter μ.

On the other hand, the indirect term generated by $N^{-1}\|\tilde{\Psi}\|^2$ is

$$-N\int \theta^{\frac{1}{2}}(x)\theta^{\frac{1}{2}}(y)\Psi(x_1,\ldots,x_{N-1},x)\Psi^\dagger(x_1,\ldots,x_{N-1},y)\times F(x,y)\,dxdydx_1\cdots dx_{N-1}, \tag{26.8.31}$$

and since the operator norm of $F(.,.,.)$ is 1, the absolute value of this term does not exceed

$$N\int \theta(x)|\Psi(x_1,\ldots,x_{N-1},x)|^2\,dx = \int\theta(x)\rho_\Psi(x)\,dx \le \int\theta(x)\rho^{\mathsf{TF}}(x)\,dx + CQ^{\frac{1}{2}}\|\nabla\theta^{\frac{1}{2}}\| \tag{26.8.32}$$

where $\rho^{\mathsf{TF}}=0$ on $\mathsf{supp}(\theta)$ and $\|\nabla\theta^{\frac{1}{2}}\|\asymp\beta^{-\frac{1}{2}}\bar{r}$.

Recall that $P'(W^{\mathsf{TF}}+\nu)=\rho^{\mathsf{TF}}$. We will take $\nu'=\nu+L$ to keep Θ_Ψ larger than all the remainders including those due to replacement W by W^{TF} and ρ by ρ^{TF} in the expression above. One can observe easily that then β should satisfy (26.8.10); let us define β and then υ by (26.8.11) and (26.8.12) respectively. Then

$$\Theta_\Psi \asymp \bigl(\upsilon^{\frac{3}{2}}+B\upsilon^{\frac{1}{2}}\bigr)\beta\bar{r}^2. \tag{26.8.33}$$

Therefore

(26.8.34) Let $h\le\epsilon_0$ (i.e. $\upsilon^{\frac{1}{2}}\beta\ge C_0$), and β,υ be defined by (26.8.11) and (26.8.12) respectively. Then expression (26.8.33) is larger than $C_0\beta^{-\frac{1}{2}}Q^{\frac{1}{2}}$ and the total expression generated by $N^{-1}\|\tilde{\Psi}\|^2$ is greater than $\epsilon\Theta$ with $\Theta=\Theta_\Psi$ defined by (26.8.33).

Now let us consider the direct terms in the right-hand expression of (26.8.22). The first of them is like in (25.6.23)

$$-\int\theta^{\frac{1}{2}}(x)\varphi(\lambda L^{-1})\,d_\lambda\bigl(H_{W+\nu',x}\theta^{\frac{1}{2}}(x)e(x,y,\lambda)\bigr)_{y=x}\,dx= \tag{26.8.35}$$

$$
\begin{aligned}
-\int \theta(x)\varphi(\lambda L^{-1})\, d_\lambda\bigl(H_{W+\nu',x} e(x,y,\lambda)\bigr)_{y=x}\, dx\\
-\frac{1}{2}\int \varphi(\lambda L^{-1})[[H_W,\theta^{\frac12}],\theta^{\frac12}]\, d_\lambda e(x,x,\lambda) \ge\\
\int \theta(x)(\nu'-\nu-\lambda)\varphi(\lambda L^{-1})\, d_\lambda e(x,x,\lambda)\, dx - C\int |\nabla\theta^{\frac12}|^2 e(x,x,\nu')dx.
\end{aligned}
$$

Observe that the absolute value of last term in the right-hand expression of (26.8.35) does not exceed $C\beta^{-1}\bar{r}^2\bigl(\upsilon^{\frac32}+B\upsilon^{\frac12}\bigr)\asymp \beta^{-2}\Theta$.

The second direct term in the right-hand expression of (26.8.22) is like in (25.6.24)

$$
\begin{aligned}
-\int \theta(x)\Bigl(\rho_\Psi * |x|^{-1} - (V-W)(x)\Bigr)F(x,x)\, dx = \\
-\mathsf{D}\bigl(\rho_\Psi-\bar{\rho},\theta(x)F(x,x)\bigr)\ge\\
-C\mathsf{D}\bigl(\rho_\Psi-\rho,\rho_\Psi-\rho\bigr)^{\frac12}\cdot \mathsf{D}\Bigl(\theta^{\frac12}F(x,x),\theta^{\frac12}F(x,x)\bigr)\Bigr)^{\frac12} \ge -CQ^{\frac12}\bar{r}^{-\frac12}\Theta,
\end{aligned}
\tag{26.8.36}
$$

provided $V-W=|x|^{-1}*\rho$ with $\mathsf{D}(\rho-\rho^{\mathsf{TF}},\rho-\rho^{\mathsf{TF}})\le CQ$.

Further, the first indirect term in the right-hand expression of (26.8.22) is like in (25.6.25)

$$
\begin{aligned}
-N\int \theta^{\frac12}(y)\Psi(x_1,\dots,x_{N-1},x)\Psi^\dagger(x_1,\dots,x_{N-1},y)\times\\
\varphi(\lambda L^{-1})\, d_\lambda\bigl(H_{W+\nu',x}\theta^{\frac12}(x)e(x,y,\lambda)\bigr)\, dxdydx_1\cdots dx_{N-1} =\\
-N\int \theta^{\frac12}(y)\theta^{\frac12}(x)\Psi(x_1,\dots,x_{N-1},x)\Psi^\dagger(x_1,\dots,x_{N-1},y)\times\\
\varphi(\lambda L^{-1})(\nu'-\nu-\lambda)\, d_\lambda e(x,y,\lambda)\, dxdydx_1\cdots dx_{N-1}\\
-N\int \theta^{\frac12}(y)\Psi(x_1,\dots,x_{N-1},x)\Psi^\dagger(x_1,\dots,x_{N-1},y)\times\\
\varphi(\lambda L^{-1})[H_{W,x},\theta^{\frac12}(x)]\, d_\lambda e(x,y,\lambda)\, dxdydx_1\cdots dx_{N-1}.
\end{aligned}
\tag{26.8.37}
$$

Observe that one can rewrite the sum of the first terms in the right-hand expressions in (26.8.35) and (26.8.37) as $\sum_j \varphi(\lambda_j L^{-1})(\nu'-\nu-\lambda_j)\|\hat{\Psi}_j\|^2$ with

$$
\hat{\Psi}_j(x_1,\dots,x_{N-1}) := \int \Psi(x_1,\dots,x_{N-1},x)\theta^{\frac12}(x)\phi_j(x)\, dx
$$

and therefore this sum is non-negative.

One can see easily that the absolute value of the second term in the right-hand expression of (26.8.37) does not exceed

$$\int \rho_\Psi(y)\theta^{\frac{1}{2}}(y)\,dy \times \beta^{-1}\int \theta_1(x)e(x,x,\nu')\,dx \asymp C\Theta \times C\bigl(\upsilon^{\frac{3}{2}}+B\upsilon\bigr)\bar{r}^2 \asymp C\beta^{-\frac{3}{2}}\bar{r}Q^{\frac{1}{2}}\Theta$$

due the choice of β. This is larger than the absolute value of the right-hand expression in (26.8.36). Therefore (cf. 25.6.26) we conclude that

(26.8.38) The sum of the first direct and indirect terms in the right-hand expression of (26.8.22) is greater than $-C\beta^{-\frac{3}{2}}\bar{r}Q^{\frac{1}{2}}\Theta$.

Finally, we need to consider the second indirect term generated by the right-hand expression of (26.8.22):

$$\begin{gathered}-\int\Bigl(\sum_{1\le i\le N}|y-x_i|^{-1}-(V-W)(y)\Bigr)\times\\ \Psi(x_1,\dots,x_N)\Psi^\dagger(x_1,\dots,x_{N-1},y)\theta^{\frac{1}{2}}(x_N)\theta^{\frac{1}{2}}(y)F(x_N,y)\,dx_1\cdots dx_N dy=\\ -\int\Bigl(|y|^{-1}*\varrho_{\underline{x}}(y)-(V-W)(y)\Bigr)\Psi(x_1,\dots,x_N)\Psi^\dagger(x_1,\dots,x_{N-1},y)\times\\ \theta^{\frac{1}{2}}(x_N)\theta^{\frac{1}{2}}(y)F(x_N,y)\,dx_1\cdots dx_N dy\\ -\int\Bigl(\sum_{1\le i\le N}|y-x_i|^{-1}-|y|^{-1}*\varrho_{\underline{x}}(y)\Bigr)\Psi(x_1,\dots,x_N)\Psi^\dagger(x_1,\dots,x_{N-1},y)\times\\ \theta^{\frac{1}{2}}(x_N)\theta^{\frac{1}{2}}(y)F(x_N,y)\,dx_1\cdots dx_N dy;\end{gathered}\tag{26.8.39}$$

recall that $\varrho_{\underline{x}}$ is a smeared density, $\underline{x}=(x_1,\dots,x_N)$.

Since $|y|^{-1}*\varrho_{\underline{x}}(y)-(V-W)(y)=|y|^{-1}*(\varrho_{\underline{x}}-\rho)$, the first term in the right-hand expression is equal to

$$\begin{gathered}\int\theta^{\frac{1}{2}}(x_N)\Psi(x_1,\dots,x_N)\times\\ \mathsf{D}_y\Bigl(\varrho_{\underline{x}}(y)-\rho(y),F(x_N,y,\lambda)\theta^{\frac{1}{2}}(y)\Psi(x_1,\dots,x_{N-1},y)\Bigr)\,dx_1\cdots dx_N\end{gathered}\tag{26.8.40}$$

and its absolute value does not exceed

(26.8.41)
$$\Bigl(N\int \mathsf{D}\bigl(\varrho_{\underline{x}}(\cdot)-\rho(\cdot),\varrho_{\underline{x}}(\cdot)-\rho(\cdot)\bigr)|\Psi(x_1,\dots,x_N)|^2\theta(x_N)\,dx_1\cdots dx_N\Bigr)^{\frac{1}{2}}\times\\
N^{-\frac{1}{2}}\Bigl(\mathsf{D}_y\Bigl(F(x_N,y,\lambda)\theta^{\frac{1}{2}}(y)\Psi(x_1,\dots,x_{N-1},y),\\
F(x_N,y,\lambda)\theta^{\frac{1}{2}}(y)\Psi(x_1,\dots,x_{N-1},y)\Bigr)\,dx_1\cdots dx_N\Bigr)^{\frac{1}{2}}.$$

Recall that the first factor is equivalently defined by (25.5.4) and therefore due to estimate (25.5.24) it does not exceed $\bigl((Q+T+\varepsilon^{-1}N)\Theta+P\bigr)^{\frac{1}{2}}$, where we assume that $\varepsilon\le Z^{-\frac{2}{3}}$ and $\Theta\asymp\beta\bigl(v^{\frac{3}{2}}+Bv^{\frac{1}{2}}\bigr)\bar{r}^2\beta\asymp\beta^{-\frac{1}{2}}\bar{r}Q^{\frac{1}{2}}$ is now an upper estimate for $\int\theta(y)\rho_\Psi(y)\,dy$-like expressions.

Then, according to (25.5.25), $P\asymp C\beta^{-2}\Theta\ll Q\Theta$ and, according to (25.5.23), $T\ll Q$ and therefore in all such inequalities we may skip P and T terms; so we get $C(Q+\varepsilon^{-1}N)^{\frac{1}{2}}\Theta^{\frac{1}{2}}$.

Meanwhile, the second factor in (26.8.41) (without square root) is equal to

$$N^{-1}\int L^{-2}\varphi'(\lambda L^{-1})\varphi'(\lambda' L^{-1})|y-z|^{-1}\underbrace{e(x_N,y,\lambda)}\theta^{\frac{1}{2}}(y)\Psi(x_1,\dots,x_{N-1},y)\times\\
\underbrace{e(x_N,z,\lambda')}\theta^{\frac{1}{2}}(z)\Psi^\dagger(x_1,\dots,x_{N-1},z)\,dydz\,dx_1\cdots dx_{N-1}\,\underbrace{dx_N}\,d\lambda d\lambda';$$

after integration with respect to x_N we get instead of the marked terms $e(y,z,\lambda)$ (recall that $e(.,.,.)$ is the Schwartz kernel of the projector and we keep $\lambda<\lambda'$) and then, integrating with respect to λ' we arrive to

$$N^{-1}\int |y-z|^{-1}F(y,z)\theta^{\frac{1}{2}}(y)\Psi(x_1,\dots,x_{N-1},y)\times\\
\theta^{\frac{1}{2}}(z)\Psi^\dagger(x_1,\dots,x_{N-1},z)\,dydz\,dx_1\cdots dx_{N-1},$$

where now F is defined by (26.8.25) albeit with φ^2 instead of φ. This latter expression does not exceed

$$N^{-1}\iint |y-z|^{-1}|F(y,z)|\theta^{\frac{1}{2}}(y)|\Psi(x_1,\dots,x_{N-1},y)|^2\times\\
dydz\,dx_1\cdots dx_{N-1}. \tag{26.8.42}$$

Then due to Proposition 26.A.6 expression $\int |y-z|^{-1}|F(y,z)|\,dz$ does not exceed $C\beta^{-1}(h^{-1}+\mu)\asymp \upsilon^{\frac{1}{2}}+B\upsilon^{-\frac{1}{2}}$, and thus expression (26.8.42) does not exceed $CZ^{-2}\bigl(\upsilon^{\frac{1}{2}}+B\upsilon^{-\frac{1}{2}}\bigr)\Theta$. Therefore the second factor in (26.8.41) does not exceed $CN^{-1}\bigl(\upsilon^{\frac{1}{4}}+B^{\frac{1}{2}}\upsilon^{-\frac{1}{4}}\bigr)\Theta^{\frac{1}{2}}$ and the whole expression (26.8.41) does not exceed

$$C(Q+\varepsilon^{-1}N)^{\frac{1}{2}}\Theta^{\frac{1}{2}}\times N^{-1}\bigl(\upsilon^{\frac{1}{4}}+B^{\frac{1}{2}}\upsilon^{-\frac{1}{4}}\bigr)\Theta^{\frac{1}{2}}=\\ CN^{-1}(Q+\varepsilon^{-1}N)^{\frac{1}{2}}\bigl(\upsilon^{\frac{1}{4}}+B^{\frac{1}{2}}\upsilon^{-\frac{1}{4}}\bigr)\Theta.$$

Finally we arrive to

Proposition 26.8.5 [48]**.** *Let*

$$\upsilon\geq \max\bigl(Z^{-\frac{4}{3}}Q^{\frac{2}{3}};\ Z^{-\frac{4}{5}}Q^{\frac{2}{5}}B^{\frac{2}{5}}\bigr) \tag{26.8.43}$$

and

$$\varepsilon\geq Z^{-1}\max(\upsilon^{-\frac{3}{2}},B\upsilon^{-\frac{5}{2}}). \tag{26.8.44}$$

Then the first term in the right-hand expression of (26.8.39) *does not exceed* $C\upsilon\Theta$.

Further, we need to estimate the second term in the right-hand expression of (26.8.39). It can be rewritten in the form

$$\sum_{1\leq i\leq N}\int U(x_i,y)\Psi(x_1,\ldots,x_N)\Psi^\dagger(x_1,\ldots,x_{N-1},y)\theta^{\frac{1}{2}}(x_N)\theta^{\frac{1}{2}}(y)\times\\ F(x_N,y)\,dx_1\cdots dx_Ndy, \tag{26.8.45}$$

where $U(x_i,y)$ is the difference between two potentials, one generated by the charge $\delta(x-x_i)$ and another by the same charge smeared; note that $U(x_i,y)$ is supported in $\{(x_i,y)\colon |x_i-y|\leq\varepsilon\}$. Let us estimate the i-th term in this sum with $i<N$ first. Multiplied by $N(N-1)$, it does not exceed

$$N\Bigl(\int |U(x_i,y)|^2|\Psi(x_1,\ldots,x_N)|^2\theta^{\frac{1}{2}}(x_N)\theta^{\frac{1}{2}}(y)|F(x_N,y)|\,dx_1\cdots dx_Ndy\Bigr)^{\frac{1}{2}}\times\\ N\Bigl(\int \omega(x_i,y)|\Psi(x_1,\ldots,x_{N-1},y)|^2\theta^{\frac{1}{2}}(x_N)\theta^{\frac{1}{2}}(y)|F(x_N,y)|\,dx_1\cdots dx_Ndy\Bigr)^{\frac{1}{2}} \tag{26.8.46}$$

[48] Cf. claim (25.6.31).

here ω is ε-admissible and supported in $\{(x_i,y)\colon |x_i-y|\le 2\varepsilon\}$ function.

Due to Proposition 26.A.6 in the second factor

$$\int \theta^{\frac12}(x_N)|F(x_N,y)|\,dx_N \le C(1+\mu h)\asymp C(1+B\upsilon^{-1})$$

and therefore the whole second factor does not exceed

$$C\Bigl(\underbrace{\int \theta^{\frac12}(x)\omega(x,y)\varrho^{(2)}_\Psi(x,y)\,dxdy}\Bigr)^{\frac12}(1+B\upsilon^{-1})^{\frac12}, \tag{26.8.47}$$

where we replaced x_i by x. According to Proposition 25.5.1 in the selected expression one can replace $\rho^{(2)}_\Psi(x,y)$ by $\rho_\Psi(x)\rho(y)$, with an error which does not exceed

$$C\Bigl(\sup_x \|\nabla_y\chi_x\|_{\mathscr{L}^2(\mathbb{R}^3)}\bigl(Q+\varepsilon^{-1}N\bigr)^{\frac12}+C\varepsilon N\|\nabla_y\chi\|_{\mathscr{L}^\infty}\Bigr)\Theta.$$

When we plug $\sup_x\|\nabla_y\chi_x\|_{\mathscr{L}^2(\mathbb{R}^3)}\asymp\varepsilon^{\frac12}$, $\|\nabla_y\chi\|_{\mathscr{L}^\infty}\asymp\varepsilon^{-1}$ this expression becomes $CN\Theta$.

Meanwhile, consider

$$\int |U(x_i,y)|^2\theta^{\frac12}(y)|F(x_N,y)|\,dy. \tag{26.8.48}$$

Again, due to Proposition 26.A.6, it does not exceed

$$C\bigl(\upsilon^{\frac32}+B\upsilon^{\frac12}\bigr)\int |U(x_i,y)|^2\theta^{\frac12}(y)\bigl(|x_N-y|\upsilon^{\frac12}+1\bigr)^{-s}\,dy$$

and this integral should be taken over $B(x_i,\varepsilon)$, with $|U(x_i,y)|\le |x_i-y|^{-1}$, so (26.8.48) does not exceed

$$C\varepsilon\bigl(\upsilon^{\frac32}+B\upsilon^{\frac12}\bigr)\omega'(x_i,x_N)$$

with $\omega'(x,y)=\bigl(1+\upsilon^{\frac12}|x-y|\bigr)^{-s}$ (provided $\varepsilon\le\upsilon^{-\frac12}$ which will be the case). Therefore the first factor in (26.8.46) does not exceed

$$C\varepsilon^{\frac12}\bigl(\upsilon^{\frac34}+B^{\frac12}\upsilon^{\frac14}\bigr)\Bigl(\underbrace{\int \theta^{\frac12}(x)\omega'(x,y)\rho^{(2)}_\Psi(x,y)\,dxdy}\Bigr)^{\frac12}. \tag{26.8.49}$$

Therefore in the selected expression one can replace $\rho^{(2)}_\Psi(x,y)$ by $\rho_\Psi(x)\rho(y)$ with an error which does not exceed what we got before but with ε replaced by $\upsilon^{-\frac{1}{2}}$, i.e. also $CN\Theta$.

However, in both selected expressions, (26.8.47) and (26.8.49), replacing $\rho^{(2)}_\Psi(x,y)$ by $\rho_\Psi(x)\rho(y)$ we get just 0. Therefore expression (26.8.46) does not exceed $C\varepsilon^{\frac{1}{2}}\bigl(\upsilon^{\frac{3}{4}}+B^{\frac{1}{2}}\upsilon^{\frac{1}{4}}\bigr)Z\Theta$, which, in turn, does not exceed $C\upsilon\Theta$ provided $\varepsilon\le C\upsilon^{\frac{1}{2}}\bigl(1+B\upsilon^{-1}\bigr)^{-1}Z^{-2}$.

So, we have two restriction to ε from above: the last one and $\varepsilon\le Z^{-\frac{2}{3}}$ and one can see easily that both of them are compatible with with restriction to ε in (26.8.43); also we can see easily that condition (26.8.43) is weaker than $\upsilon\ge\bigl\{Z^{\frac{20}{21}}:Z^{\frac{20}{27}}B^{\frac{2}{9}}:Z^{\frac{4}{15}}B^{\frac{26}{45}}\bigr\}$ if $\bigl\{B\le Z^{\frac{20}{21}};\,Z^{\frac{20}{21}}\le B\le Z^{\frac{4}{3}};\,Z^{\frac{4}{3}}\le B\le Z^{3}\bigr\}$ respectively.

Finally, consider term in (26.8.45) with $i=N$ (multiplied by N):

$$N\int U(x_N,y)|\Psi(x_1,\ldots,x_N)|^2\theta^{\frac{1}{2}}(x_N)\theta^{\frac{1}{2}}(y)F(x_N,y)\,dx_1\cdots dx_Ndy \tag{26.8.50}$$

due to Cauchy inequality it does not exceed

$$\begin{aligned}N\Bigl(\int |x_N-y|^{-2}|\Psi(x_1,\ldots,x_N)|^2\theta^{\frac{1}{2}}(x_N)\theta^{\frac{1}{2}}(y)\ dx_1\cdots dx_Ndy\Bigr)^{\frac{1}{2}}\times\\ N\Bigl(\int |F(x_N,y)|^2|\Psi(x_1,\ldots,x_N)|^2\theta^{\frac{1}{2}}(x_N)\theta^{\frac{1}{2}}(y)\ dx_1\cdots dx_Ndy\Bigr)^{\frac{1}{2}}\end{aligned} \tag{26.8.51}$$

where both integrals are taken over $\{|x_N-y|\le\varepsilon\}$. Integrating with respect to y there we get that it that it does not exceed

$$C\varepsilon^{\frac{1}{2}}\Theta^{\frac{1}{2}}\times\bigl(\upsilon^{\frac{3}{4}}+B\upsilon^{\frac{1}{4}}\bigr)\varepsilon^{\frac{3}{2}}\Theta^{\frac{1}{2}}=C\bigl(\upsilon^{\frac{3}{4}}+B\upsilon^{\frac{1}{4}}\bigr)\varepsilon^2\Theta\ll\upsilon\Theta.$$

Therefore the right-hand expression in (26.8.22) is $\ge -C\upsilon\Theta$ and recalling that $\nu'-\nu=O(\upsilon)$ we recover a lower estimate $\mathsf{I}_N+\nu\ge -C\upsilon$ in Theorem 26.8.6 below. Here υ must be found from (26.8.11)–(26.8.12) and must satisfy $\upsilon\le|\nu|$.

Combining this estimate with the estimate from the above, derived in Proposition 26.8.3 we arrive to

Theorem 26.8.6. *Let $M=1$. Let condition* (26.2.28) *be fulfilled. Then*

(i) For $B\le Z^{\frac{20}{21}}$ and $|\nu|\ge Z^{\frac{20}{21}}$

$$|\mathsf{I}_N+\nu|\le CZ^{\frac{5}{18}}|\nu|^{\frac{17}{24}}. \tag{26.8.52}$$

(ii) For $Z^{\frac{20}{21}} \le B \le Z^{\frac{4}{3}}$ *and* $|\nu| \ge Z^{\frac{20}{27}} B^{\frac{2}{9}}$ *estimate* (26.8.17) *from above and estimate*

$$\mathsf{I}_N + \nu \ge -C \begin{cases} Z^{\frac{5}{18}} |\nu|^{\frac{17}{24}} & \text{if } B \le Z^{\frac{5}{18}} |\nu|^{\frac{17}{24}}, \\ Z^{\frac{5}{12}} B^{-\frac{1}{2}} |\nu|^{\frac{17}{16}} & \text{if } Z^{\frac{5}{18}} |\nu|^{\frac{17}{24}} \le B \le |\nu|, \\ Z^{\frac{5}{12}} B^{-\frac{3}{16}} |\nu|^{\frac{3}{4}} & \text{if } |\nu| \le B \le Z^{-\frac{20}{7}} |\nu|^4, \\ Z^{\frac{20}{21}} & \text{if } Z^{-\frac{20}{7}} |\nu|^4 \le B \end{cases} \tag{26.8.53}$$

from below hold.

(iii) For $Z^{\frac{20}{21}} \le B \le Z^3$ *and* $|\nu| \ge Z^{\frac{4}{15}} B^{\frac{26}{45}}$ *estimate* (26.8.19) *from above and estimate*

$$\upsilon = \begin{cases} Z^{-\frac{1}{10}} B^{\frac{1}{5}} |\nu|^{\frac{3}{4}} & \text{if } B \le Z^{-\frac{1}{2}} |\nu|^{\frac{1}{4}} \\ Z^{\frac{4}{35}} B^{\frac{22}{35}} & \text{if } Z^{-\frac{1}{2}} |\nu|^{\frac{1}{4}} \le B \end{cases} \tag{26.8.54}$$

from below hold.

Remark 26.8.7. Recall that $Q = Z^{\frac{5}{3}} \bigl(B^{\delta} + 1\bigr) Z^{-\delta}$ as $B \le Z$; therefore we can add factor $\bigl(B^{\delta'} + 1\bigr) Z^{-\delta'}$ in all estimates of Theorem 26.8.6.

26.8.3 Estimates for Ionization Energy: $M \ge 2$

Recall that for $M \ge 2$ we have only estimate (26.6.73):

$$\mathsf{D}(\rho_\Psi - \rho,\, \rho_\Psi - \rho \le \bar{Q}) \coloneqq (26.5.40) + (26.6.69).$$

Then exactly the same arguments lead us to the following (we leave all details to the reader):

Theorem 26.8.8. *Let* $M \ge 2$*. Then*

(i) Estimate $\mathsf{I}_N + \nu \le C(\upsilon + \varsigma)$ *holds with* υ *and* ς *defined by* (26.8.11)–(26.8.12) *and* (26.8.13) *albeit with* Q *replaced by* $\bar{Q}$*.*

(ii) Estimate $\mathsf{I}_N + \nu \ge -C\upsilon$ *holds with* υ *defined by* (26.8.11)–(26.8.12) *albeit with* Q *replaced by* $\bar{Q}$*.*

Therefore the case when $\bar{Q} \le Q$ is not affected. One can see easily that it happens for sure as $B \le Z^{\frac{20}{17}} L^{-\kappa}$ where $\kappa > 0$ is some exponent.

We leave to the reader

Problem 26.8.9. (i) Find explicit formula for $\upsilon + \varsigma$ and υ.

(ii) Find $\nu^* = \nu^*(Z, B)$ and $\nu_* = \nu_*(Z, B)$ such that $|\nu| \lesssim \upsilon + \varsigma$ iff and only if $\nu \lesssim \nu^*$ and $|\nu| \lesssim \upsilon$ iff and only if $\nu \lesssim \nu_*$.

26.8.4 Free Nuclei Model

In this subsection we consider two extra problems appearing in the free nuclei model–estimate the minimal distance between nuclei and the maximal excessive positive charge when system does not break apart. We also slightly improve estimates for the maximal negative charge and for the ionization energy.

Preliminary Arguments

Recall that we assume that

$$\mathsf{Q} := \hat{\mathsf{E}} - \sum_{1\le m\le M} \mathsf{E}_m < 0 \tag{26.8.55}$$

where

$$\hat{\mathsf{E}} = \mathsf{E} + \sum_{1\le m<m'\le M} \frac{Z_m Z_{m'}}{|\mathsf{y}_m - \mathsf{y}_{m'}|}. \tag{26.8.56}$$

We apply estimate from below for $\hat{\mathsf{E}}$ delivered by Proposition 26.6.1(ii), and estimates from above for E_m, delivered by Theorem 26.6.6(ii); then

$$\hat{\mathcal{E}}^{\mathsf{TF}} + \mathsf{Scott} - \sum_{1\le m\le M} \Bigl(\mathcal{E}_m^{\mathsf{TF}} - \mathsf{Scott}_m\Bigr) \le CQ + CZ^{\frac{4}{3}} B^{\frac{1}{3}} + Ca^{-\frac{1}{2}} Z^{\frac{3}{2}}$$

or, equivalently, due to equality $\mathsf{Scott} = \sum_{1\le m\le M} \mathsf{Scott}_m$ and non-binding theorem

$$0 \le \mathcal{Q} := \hat{\mathcal{E}}^{\mathsf{TF}} - \sum_{1\le m\le M} \mathcal{E}_m^{\mathsf{TF}} \le CQ + CZ^{\frac{4}{3}} B^{\frac{1}{3}} + Ca^{-\frac{1}{2}} Z^{\frac{3}{2}}. \tag{26.8.57}$$

Assume that assumption (26.2.28) is fulfilled. Then $\mathcal{Q} \asymp \mathcal{E}^{\mathsf{TF}}$ for $a \le \epsilon r^*$ with $r^* = \min(Z^{-\frac{1}{3}};\, B^{-\frac{2}{5}} Z^{\frac{1}{5}})$ and therefore

(26.8.58) In the free nuclei model $a \ge \epsilon r^*$.

Then the last term in (26.8.57) is not needed.

Remark 26.8.10. (i) Obviously, the second term $CZ^{\frac{4}{3}}B^{\frac{1}{3}}$ in the right-hand expression of (26.8.57) matters only if $Z \le B \le Z^{\frac{11}{7}}$; however we will show that it could be skipped even in this case.

(ii) If $B \le Z$ we can replace the right-hand expression of (26.8.57) by $Z^{\frac{5}{3}-\delta}(1+B^{\delta})$.

(iii) All these estimates hold also for $\mathsf{D}(\rho_\Psi-\rho^{\mathsf{TF}},\rho_\Psi-\rho^{\mathsf{TF}})$ because this term is present in the estimate from below.

Minimal Distance

We are going to improve (26.8.58). Consider the case $B \le Z^{\frac{4}{3}}$ first. Then since $\mathcal{Q} \ge \epsilon_0 a^{-7}$ for $\epsilon r^* \le a \le \epsilon \bar{r}$ (where in this case $r^* = Z^{-\frac{1}{3}} \le \bar{r} = B^{-\frac{1}{4}}$), we conclude that $a \gtrsim Z^{-\frac{5}{21}}$ provided $B \le Z^{\frac{20}{21}}$.

Furthermore, then we can apply improved remainder estimate $O(Z^{\frac{5}{3}-\delta})$, since the difference between Dirac–Schwinger terms for a molecule and the sum of these terms for the atoms is also $O(Z^{\frac{5}{3}-\delta})$ as long as $a \ge Z^{-\frac{1}{3}+\delta_1}$, which is the case. Then we conclude that $a \ge Z^{-\frac{5}{21}-\delta'}$ as long as it is less than $\epsilon\bar{r}$ and we arrive to Statement (i) of Proposition 26.8.11:

Proposition 26.8.11. *Let condition* (26.2.28) *be fulfilled. Then in the free nuclei model*

(i) For $B \le Z^{\frac{20}{21}}$ the minimal distance satisfies

$$a \ge \min(Z^{-\frac{5}{21}-\delta}, \epsilon B^{-\frac{1}{4}}). \tag{26.8.59}$$

(ii) For $Z^{\frac{20}{21}} \le B \le Z^3$ the distances satisfy

$$|\mathsf{y}_m - \mathsf{y}_{m'}| \ge \bar{r}_m + \bar{r}_{m'} - \epsilon\bar{r} \qquad \forall m \ne m' \tag{26.8.60}$$

with arbitrarily small constant $\epsilon > 0$ where $\bar{r}_m$ denote the exact radii of $\mathsf{supp}(\rho_m^{\mathsf{TF}})$.

Proof. We need to prove Statement (ii). Observe that it also follows from the arguments above in the case $Z^{\frac{20}{21}} \le B \le Z$.

For $Z\le B\le CZ^{\frac{4}{3}}$ the remainder estimate is $O(Z^{\frac{4}{3}}B^{\frac{1}{3}})$ and the same arguments imply that $|\mathsf{y}_m-\mathsf{y}_{m'}|\ge \epsilon Z^{-\frac{4}{21}}B^{-\frac{1}{21}}$ unless $a\ge\epsilon\bar{r}$ and since the latter is weaker, it must be satisfied. Therefore if (26.8.60) fails, then in virtue of Theorem 26.2.17 $\mathcal{Q}\ge\epsilon_1 B^{\frac{7}{4}}$, which is larger than the remainder estimate $CZ^{\frac{4}{3}}B^{\frac{1}{3}}$.

Finally, case $C_\epsilon Z^{\frac{4}{3}}\le B\le Z^3$ follows from the fact that if (26.8.60) fails then in virtue of Theorem 26.2.17 $\mathcal{Q}\ge\epsilon_1 Z^{\frac{9}{5}}B^{\frac{2}{5}}$. □

Proposition 26.8.12. *Let condition* (26.2.28) *be fulfilled. Then in the free nuclei model*

$$\mathcal{Q}+\mathsf{D}(\rho_\Psi-\rho^{\mathsf{TF}},\,\rho_\Psi-\rho^{\mathsf{TF}})\le CQ. \tag{26.8.61}$$

Proof. We need to cover only case $Z\le B\le Z^{\frac{11}{7}}$, since only in this case term $CZ^{\frac{4}{3}}B^{\frac{1}{3}}$ matters.

We apply now estimate from below for $\hat{\mathsf{E}}$ delivered by Proposition 26.6.1(i), and estimates from above for E_m, delivered by Theorem 26.6.6(i); then we do not have term $CZ^{\frac{4}{3}}B^{\frac{1}{3}}$ but instead of equal to 0 difference of the Scott correction terms, we get

$$\Bigl(\operatorname{Tr}((H_{A,W}-\nu)^-)+\int P_B(W^{\mathsf{TF}}+\nu)\,dx\Bigr)-\\ \sum_{1\le m\le M}\Bigl(\operatorname{Tr}((H_{A,W_m}-\nu')^-)+\int P_B(W^{\mathsf{TF}}+\nu')\,dx\Bigr), \tag{26.8.62}$$

where we know that $\nu'=\nu_1=...=\nu_M$.

Let us use partition of unity $\phi_0+\phi_1+...+\phi_M=1$ where $\phi_m=1$ in $B(\mathsf{y}_m,\epsilon\bar{r}_m)$ and is supported in $B(\mathsf{y}_m,2\epsilon\bar{r}_m)$. Then our standard methods imply that the absolute values of

$$\operatorname{Tr}\bigl((H_{A,W}-\nu)^-\phi_0\bigr)+\int P_B(W^{\mathsf{TF}}+\nu)\phi_0(x)\,dx, \tag{26.8.63}$$

and

$$\operatorname{Tr}\bigl((H_{A,W_m}-\nu')^-\phi_{m'}\bigr)+\int P_B(W_m^{\mathsf{TF}}+\nu')\phi_{m'}\,dx \tag{26.8.64}$$

with $m=1,\dots,M$, $m'=0,1,\dots,M$, $m'\ne m$ do not exceed CQ [49]. Therefore we need to estimate an absolute value of

$$\mathsf{Tr}\Bigl(\bigl[(H_{A,W}-\nu)^- - (H_{A,W_m}-\nu')^-\bigr]\phi_m\Bigr)+ \int \bigl(P_B(W^{\mathsf{TF}}+\nu)-P_B(W^{\mathsf{TF}}_m+\nu')\bigr)\phi_m\,dx. \tag{26.8.65}$$

Due to Proposition 26.8.11 $B(\mathsf{y}_m,3\epsilon\bar r)$ does not intersect $B(\mathsf{y}_{m'},\bar r_{m'})$ and then in $B(\mathsf{y}_m,3\epsilon\bar r)$ $W_{m'}\le C(Z-N)\bar r^{-1}$. Using this inequality and

$$\mathsf{D}(\rho-\rho_1-\dots-\rho_M,\,\rho-\rho_1-\dots-\rho_M)\le C\mathcal{Q}, \tag{26.8.66}$$

one can prove easily that there also

$$|W-W_m|\le CT\coloneqq C\mathcal{Q}^{\frac12}\bar r^{-\frac12}+C(Z-N)\bar r^{-1} \tag{26.8.67}$$

and, moreover,

$$|\nabla(W-W_m)|\le CT\bar r^{-1}=C\mathcal{Q}^{\frac12}\bar r^{-\frac32}+C(Z-N)\bar r^{-2}, \tag{26.8.68}$$

$$|\nabla^2(W-W_m)|\le CT\bar r^{-2}=C\mathcal{Q}^{\frac12}\bar r^{-\frac52}+C(Z-N)\bar r^{-3}. \tag{26.8.69}$$

Then using our standard methods one can prove easily that an absolute value of expression (26.8.65) with ϕ_m replaced by ℓ-admissible function ψ_m does not exceed

$$CTh^{-2}(1+\mu h) \tag{26.8.70}$$

with our standard

$$h=Z^{-\frac12}r^{-\frac12},\qquad \mu=BZ^{-\frac12}r^{\frac32} \tag{26.8.71}$$

if <u>either</u> $B\le Z^{\frac43}$, $r\le r^*Z^{-\frac13}$ <u>or</u> $Z^{\frac43}\le B\le Z^3$, $r\le\bar r$ and

$$h=r,\qquad \mu=Br^3 \tag{26.8.72}$$

if $B\le Z^{\frac43}$. Plugging (26.8.71) and (26.8.72) and summing over partition we arrive to $CTZ^{\frac23}$ as $Z^{\frac{20}{21}}\le B\le Z^{\frac43}$ and $CTZ^{\frac25}B^{\frac15}$ as $Z^{\frac43}\le B\le Z^3$.

Plugging $T=(Z-N)\bar r^{-1}$ we get expressions which are much smaller than $\epsilon(Z-N)^2\bar r^{-1}$ due to (26.8.61); plugging $T=\mathcal{Q}^{\frac12}\bar r^{-\frac12}$ we get terms smaller than $\epsilon'\mathcal{Q}+C(\epsilon')B^{\frac14}Z^{\frac43}$ if $B\le Z^{\frac43}$ and $\epsilon'\mathcal{Q}+C(\epsilon')Z^{\frac35}B^{\frac45}$ if $Z^{\frac43}\le B\le Z^3$; here $\epsilon'>0$ is arbitrarily small and thus term (26.8.65) does not make any difference. □

[49] Recall that W and W_m are approximations to W^{TF} and W^{TF}_m.

Since $\mathcal{Q} \ge \epsilon a^{-1}(Z-N)^2$ we arrive to

Corollary 26.8.13. *Let condition* (26.2.28) *be fulfilled. Then*

(i) If $(Z-N) \ge C(Qa)^{\frac{1}{2}}$ where Q is our remainder estimate in the ground state energy, then in free nuclei model minimal distance between nuclei must be at least a.

(ii) In particular, if $(Z-N) \ge C_1(Q\bar{r})^{\frac{1}{2}}$ then in free nuclei model minimal distance between nuclei must be at least $C_0\bar{r}$ and molecule consists of separate atoms.

We leave to the reader

Problem 26.8.14. Using Theorem 26.2.17 and the arguments used in the proof of Proposition 26.8.11, estimate overlapping of balls $B(\mathsf{y}_m, \bar{r}_m)$ if $Z^{-\frac{5}{21}-\delta} \ge \epsilon B^{-\frac{1}{4}}$ in the free nuclei model with $N=Z$ and prove that

$$(\bar{r}_m + \bar{r}_{m'} - |\mathsf{y}_m - \mathsf{y}_{m'}|) \le C\bar{r}(K^{-2}\bar{r}^{-1}Q)^{\frac{1}{2}} = C\begin{cases} B^{-\frac{1}{4}}\bigl(B^{-\frac{7}{4}}Z^{\frac{5}{3}} + B^{-\frac{1}{2}}L\bigr)^{\frac{1}{12}} & \text{if } Z^{\frac{20}{21}} \le B \le Z^{\frac{4}{3}},\\ B^{-\frac{7}{15}}Z^{\frac{1}{10}}L^{\frac{1}{6}} & \text{if } Z^{\frac{4}{3}} \le B \le Z^3. \end{cases} \tag{26.8.73}$$

Estimate of Excessive Positive Charge

To estimate excessive positive charge when molecules can still exist in free nuclei model we apply arguments of section 5 of B. Ruskai and J. P. Solovej [1]. In view of Corollary 26.8.13 for $(Z-N)$ violating (26.8.76) below it is sufficient to assume that (25.6.41) is satisfied:

$$a = \min_{j<k} |\mathsf{y}_j - \mathsf{y}_k| \ge C_0\bar{r} \tag{26.8.74}$$

i.e. in Thomas-Fermi theory ρ^{TF} is supported in the separate "atoms". Really, it is the case if $C_0Z^{\frac{20}{21}} \le B \le Z^3$ but also it is so if $B \le C_0Z^{\frac{20}{21}}$ and $(Z-N)_+ \ge C_1Z^{\frac{5}{7}}$ since then $\bar{r} \asymp (Z-N)_+^{-\frac{1}{3}}$.

Like in Subsection 25.6.3 consider a-admissible functions $\theta_m(x)$, supported in $B(\mathsf{y}_m, \frac{1}{3}a)$ as $m=1,\dots,M$ and in $\{|x-\mathsf{y}_{m'}| \ge \frac{1}{4}a \ \ \forall m'=1,\dots,M\}$ as $m=0$, such that

$$\theta_0^2 + \dots + \theta_M^2 = 1. \tag{26.8.75}$$

Then for the ground state Ψ equality (25.6.43) holds with *cluster Hamiltonians* H_{α_m} defined by (25.6.44) and satisfying (25.6.45) and with the *intercluster Hamiltonian* J_α defined by (25.6.46) and satisfying (25.6.47) with J_{ml} defined by (25.6.48)–(25.6.49). Furthermore, equality (25.6.50) holds.

Applying Proposition 25.5.1 and estimate (25.4.56) (replacing first θ_k with $k=1,\dots,M$ by $\tilde{\theta}_k$, supported in $B(\mathsf{y}_k, c\bar{r})$, and estimating the resulting error), we conclude that (25.6.51)–(25.6.54) hold with $Y = Q^{\frac{1}{2}}\bar{r}^{\frac{1}{2}}$ since $\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}}, \rho_\Psi - \rho^{\mathsf{TF}}) \le CQ$.

The last term in (25.6.51) is estimated by Proposition 25.5.1 and estimate (26.8.61) instead of (25.4.56) and the same replacement trick; so we arrive to (25.6.55) and repeating the same trick we get that it is larger than (25.6.56).

Again let us note that the absolute value of the last term in the right-hand expression of (25.6.43) does not exceed $Ca^{-2}Y$ due to (25.6.52). Now stability condition yields that (26.6.61) must be fulfilled.

Then we conclude that (25.6.57) and (25.6.59) hold with J_{ml} defined by (25.6.58) provided (25.6.60) is fulfilled as $|x-\mathsf{y}_k| \ge C\bar{r}$.

This inequality, (26.8.74) and Proposition 25.6.6 (which is the special case of Theorem 26.2.13) yield that $Z - N \le CY = C\bar{r}^{\frac{1}{2}}Q^{\frac{1}{2}}$. Now we need to consider two cases:

(a) $B \le (Z-N)^{\frac{4}{3}}$; then $\bar{r} \asymp (Z-N)^{-\frac{1}{3}}$ and we conclude that $(Z-N) \le CQ^{\frac{3}{5}}$ exactly like in Subsubsection 25.6.3.

(b) $(Z-N)^{\frac{4}{3}} \le B \le Z^3$; then plugging $\bar{r}$ and Q we arrive to two other cases of (26.8.76).

Then we arrive to Statement (i) below; Statement (ii) follows from Remark 26.8.10(ii).

Theorem 26.8.15 [50]**.** *Let condition* (26.2.28) *be fulfilled.*

(i) Then in the framework of the free nuclei model with $M \ge 2$ the stable molecule does not exist unless

$$(Z-N)_+ \le C_1 \begin{cases} Z^{\frac{20}{21}} & \text{if } B \le Z^{\frac{20}{21}},\\ Z^{\frac{5}{6}}B^{-\frac{1}{8}} & \text{if } Z^{\frac{20}{21}} \le B \le Z^{\frac{4}{3}},\\ Z^{\frac{2}{5}}B^{\frac{1}{5}} & \text{if } Z^{\frac{4}{3}} \le B \le Z^{3}. \end{cases} \tag{26.8.76}$$

[50] Cf. Theorem 25.6.4.

(ii) Furthermore, for $B \le Z$ in the framework of the free nuclei model with $M \ge 2$ the stable molecule does not exist unless

$$(Z-N)_+ \le C_1 \begin{cases} Z^{\frac{20}{21}-\delta} & \text{if } B \le Z^{\frac{20}{21}}, \\ Z^{\frac{5}{6}-\delta} B^{-\frac{1}{8}+\delta} & \text{if } Z^{\frac{20}{21}} \le B \le Z. \end{cases} \tag{26.8.77}$$

Estimate for Excessive Negative Charge and Ionization Energy

Estimate (26.8.61) and Remark 26.8.10 immediately imply

Theorem 26.8.16. *Let condition* (26.2.28) *be fulfilled.*

(i) Then in the framework of the free nuclei model with $M \ge 2$ estimates (26.7.21) *for the excessive negative charge and* (26.7.37) *for the ionization energy $\hat{\mathsf{I}}_N = -\hat{\mathsf{E}}_N + \hat{\mathsf{E}}_{N-1}$ hold.*

(ii) Furthermore, if $B \le Z$ estimates (26.7.22) *for the excessive negative charge and* (26.7.39) *for the ionization energy $\hat{\mathsf{I}}_N$ hold.*

26.A Appendices

26.A.1 Electrostatic Inequalities

There are two kinds of electrostatic inequalities: those which hold for any fermionic state Ψ and those which hold only for the ground-state (or near ground state) Ψ. Inequalities of the first kind do not depend on the quantum Hamiltonian and they are (25.2.1) repeated here:

$$\sum_{1\le j<k\le N} \int |x_j - x_k|^{-1} |\Psi(x_1,\dots,x_N)|^2\, dx_1\cdots dx_N \ge \frac{1}{2}\mathsf{D}(\rho_\Psi,\rho_\Psi) - C\int \rho_\Psi^{\frac{4}{3}}(x)\,dx \tag{26.A.1}$$

and (26.A.5) below.

Inequalities of the second kind are for $B=0$:

$$\sum_{1\le j<k\le N} \int |x_j - x_k|^{-1} |\Psi(x_1,\dots,x_N)|^2\, dx_1\cdots dx_N \ge \frac{1}{2}\mathsf{D}(\rho_\Psi,\rho_\Psi) - CZ^{\frac{5}{3}}, \tag{26.A.2}$$

and more precise one (26.A.26) below.

For $\vec{B}=\mathsf{const}$ there is an inequality established in E. Lieb, J. P. Solovej and J. Yngvason [3] (p. 122):

Theorem 26.A.1. *Let $\vec{B}=\mathsf{const}$. Then for the ground state Ψ*

$$\int \rho_\Psi^{\frac{4}{3}}\,dx \le CZ^{\frac{5}{6}}N^{\frac{1}{2}}(Z+N)^{\frac{1}{3}}\bigl(1+BZ^{-\frac{4}{3}}\bigr)^{\frac{2}{5}}; \tag{26.A.3}$$

In particular, for $c^{-1}N\le Z\le cN$ the right-hand expression does not exceed

$$CZ^{\frac{5}{3}}\bigl(1+BZ^{-\frac{4}{3}}\bigr)^{\frac{2}{5}} \asymp C\begin{cases} Z^{\frac{5}{3}} & \textit{if}\ \ B\le Z^{\frac{4}{3}},\\ Z^{\frac{17}{15}}B^{\frac{2}{5}} & \textit{if}\ \ B\ge Z^{\frac{4}{3}}.\end{cases} \tag{26.A.4}$$

We want to establish inequality, similar to (25.A.2), but in the magnetic case. We will use for this the following

Theorem 26.A.2 [51]**.** *Fix $0<\delta\le 1/6$. Then for any density matrix F and any density $\rho_0(x)\ge 0$ the following inequality holds*

$$\begin{aligned}\sum_{1\le j<k\le N}\int |x_j-x_k|^{-1}|\Psi(x_1,\dots,x_N)|^2\,dx_1\cdots dx_N \ge{}&\\ \mathsf{D}(\rho_0,\rho_\gamma)-\frac{1}{2}\mathsf{D}(\rho_0,\rho_0)-\frac{1}{2}\sum_{\varsigma,\varsigma'}\iint |F(x,\varsigma;y,\varsigma')|^2|x-y|^{-1}\,dxdy&\\ -C\|\rho\|_{5/3}^{5/6}\cdot\|\rho\|_1^{1/6+\delta}\cdot\upsilon(\gamma,F)^{1/3-\delta},&\end{aligned} \tag{26.A.5}$$

where $\rho=\rho_0+\rho_F+\rho_\Psi$, $\upsilon(\gamma,F)\coloneqq\mathsf{Tr}(\gamma(I-F))$ and

$$\gamma=\gamma_\Psi(x,y)=N\int \Psi(x,x_2,\dots,x_N)\Psi^\dagger(y,x_2,\dots,x_N)\,dx_2\cdots x_N \tag{26.A.6}$$

is two-point one particle density.

Recall that $\|.\|_p$ denotes $\mathscr{L}^p$-norm.

There is a connection between (26.A.1) and (26.A.5): if we set $F=0$, we get $\varsigma=\|\rho\|_1$ and the last term in (26.A.5) becomes $\|\rho\|_{5/3}^{5/6}\cdot\|\rho\|_1^{1/2}$. On

[51] Lemma 6 of G. Graf and J. P. Solovej [1].

the other hand, $\|\rho\|_{4/3}^{4/3} \le \|\rho\|_{5/3}^{5/6}\cdot\|\rho\|_1^{1/2}$, so (26.A.5) is slightly deteriorated (26.A.1) with $F=0$ but with "free" ρ_0.

Let us follow G. Graf and J. P. Solovej [1] further albeit in the case of magnetic field. Let us estimate first $\|\rho\|_{5/3}$.

If $\rho=\rho^{\mathsf{TF}}$ direct calculations show that for $N\asymp Z$

$$\int \rho^{\mathsf{TF}}\,dx = \min(Z,N), \tag{26.A.7}$$

$$\int (\rho^{\mathsf{TF}})^{\frac{4}{3}}\,dx \asymp C\rho^{*\,\frac{4}{3}}r^{*\,3} = CZ^{\frac{5}{3}}\bigl(1+BZ^{-\frac{4}{3}}\bigr)^{\frac{2}{5}}, \tag{26.A.8}$$

$$\int (\rho^{\mathsf{TF}})^{\frac{5}{3}}\,dx \asymp C\rho^{*\,\frac{5}{3}}r^{*\,3} = CZ^{\frac{7}{3}}\bigl(1+BZ^{-\frac{4}{3}}\bigr)^{\frac{4}{5}} \tag{26.A.9}$$

with

$$r^* = \min(Z^{-\frac{1}{3}}, B^{-\frac{2}{5}}Z^{\frac{1}{5}}) \asymp Z^{-\frac{1}{3}}\bigl(1+BZ^{-\frac{4}{3}}\bigr)^{-\frac{2}{5}}, \tag{26.A.10}$$

$$\rho^* = \min(N,Z)r^{*\,-3} \tag{26.A.11}$$

and we use $\|\rho\|_{5/3}^{5/6}\cdot\|\rho\|_1^{1/2} \asymp \|\rho\|_{4/3}^{4/3}$ for $\rho=\rho^{\mathsf{TF}}$.

If $\rho=\rho_\Psi$ we use magnetic Lieb–Thirring inequality (see f.e. Theorem 2.2 in L. Erdös [1])

$$\mathsf{Tr}(H^-_{A,W}) \ge -C\int P_B(W)\,dx \tag{26.A.12}$$

and therefore

$$\begin{aligned}\langle \mathsf{H}\Psi,\Psi\rangle \ge \mathsf{Tr}((H_{A,W})^-) + \int W\rho_\Psi\,dx \\ - \int V\rho_\Psi\,dx + \frac{1}{2}\mathsf{D}(\rho_\Psi,\rho_\Psi) - C\|\rho_\Psi\|_{4/3}^{4/3},\end{aligned} \tag{26.A.13}$$

which due to (26.A.12) is greater than

$$\begin{aligned}\int \bigl(-CP_B(W)+W\rho_\Psi\bigr)\,dx - \\ \int V\rho_\Psi\,dx + \frac{1}{2}\mathsf{D}(\rho_\Psi,\rho_\Psi) - C\|\rho_\Psi\|_{4/3}^{4/3} \ge \\ 3\epsilon_0\int \tau_B(\rho_\Psi)\,dx - \int V\rho_\Psi\,dx + \frac{1}{2}\mathsf{D}(\rho_\Psi,\rho_\Psi) - C\|\rho_\Psi\|_{4/3}^{4/3}\end{aligned} \tag{26.A.14}$$

where we picked up $W : CP'_B(W) = \rho_\Psi$.

The first two terms in the right-hand expression are estimated from below by

$$2\epsilon_0 \int \tau_B(\rho_\Psi)\,dx - C\int P_B(V)\phi\,dx - C\int V\rho_\Psi(1-\phi)\,dx,$$

where $\mathsf{supp}(\phi)\subset\{x\colon \ell(x)\le 2r^*\}$ and $\mathsf{supp}(1-\phi)\subset\{x\colon \ell(x)\ge r^*\}$.

One can see easily that the absolute value of the second term is $\asymp Z^{\frac{7}{3}}\bigl(1+BZ^{-\frac{4}{3}}\bigr)^{\frac{2}{5}}$, while the absolute value of the third term does not exceed $CZ\int V(1-\phi)\,dx \asymp CZ^2 r^{*\,-1}$ which does not exceed the same expression $Z^{\frac{7}{3}}\bigl(1+BZ^{-\frac{4}{3}}\bigr)^{\frac{2}{5}}$. Therefore

$$\langle \mathsf{H}\Psi,\Psi\rangle + C_1 Z^{\frac{7}{3}}\bigl(1+BZ^{-\frac{4}{3}}\bigr)^{\frac{2}{5}} \ge 2\epsilon_0\int \tau_B(\rho_\Psi)\,dx + \frac{1}{2}\mathsf{D}(\rho_\Psi,\rho_\Psi) - C\|\rho_\Psi\|_{4/3}^{4/3}. \tag{26.A.15}$$

Note that $\|\rho_\Psi\|_{4/3}^{4/3}$, calculated over domain $\{x\colon \rho_\Psi(x)\ge B^{\frac{4}{3}}\}$, does not exceed $C\|\rho_\Psi\|_{5/3}^{5/6}\cdot\|\rho\|_1^{\frac{1}{2}}$ with norms, calculated over the same domain, which does not exceed $CT^{\frac{1}{2}}Z^{\frac{1}{2}}$ with $T=\int\tau_B(\rho_\Psi)\,dx$.

Meanwhile, $\|\rho_\Psi\|_{4/3}^{4/3}$, calculated over domain $\{x\colon \rho_\Psi(x)\le B^{\frac{4}{3}}\}$, does not exceed $C\|\rho\|_3^{\frac{1}{2}}\cdot\|\rho\|_1^{\frac{5}{6}}$ with norms, calculated over the same domain, which does not exceed $CZ^{\frac{1}{2}}B^{\frac{1}{3}}T^{\frac{1}{6}}$.

Therefore

$$\|\rho_\Psi\|_{4/3}^{4/3} \le CT^{\frac{1}{2}}Z^{\frac{1}{2}} + CZ^{\frac{5}{6}}B^{\frac{1}{3}}T^{\frac{1}{6}} \tag{26.A.16}$$

and therefore (26.A.15) implies that if

$$\langle \mathsf{H}\Psi,\Psi\rangle \le C_1 Z^{\frac{7}{3}}\bigl(1+BZ^{-\frac{4}{3}}\bigr)^{\frac{2}{5}}, \tag{26.A.17}$$

then

$$T=\int \tau_B(\rho_\Psi)\,dx \le C_2 Z^{\frac{7}{3}}\bigl(1+BZ^{-\frac{4}{3}}\bigr)^{\frac{2}{5}} \tag{26.A.18}$$

and

$$\|\rho_\Psi\|_{4/3}^{4/3} \le CZ^{5/3}\bigl(1+BZ^{-\frac{4}{3}}\bigr)^{\frac{2}{5}}; \tag{26.A.19}$$

taking $F=0$ we arrive to (26.A.3) if $N\asymp Z$.

However, on our preparatory step we need to estimate also $\|\rho_\Psi\|_{5/3}^{5/3}$ and due to (26.A.18) we need to consider only norms over $\{x\colon \rho_\Psi(x)\ge B^{\frac{4}{3}}\}$. Then $\|\rho_\Psi\|_{5/3}^{5/3}\le C\|\rho_\Psi\|_{4/3}^{16/15}\cdot \|\rho_\Psi\|_3^{3/5}$ and plugging the same estimates (26.A.19), (26.A.19) we conclude that

$$\|\rho_\Psi\|_{5/3}^{5/3}\le CZ^{7/3}\bigl(1+BZ^{-\frac{4}{3}}\bigr)^{\frac{4}{5}}. \tag{26.A.20}$$

Now we assume that $B\le Z^3$, take $F=e(x,y,\nu)$, where $e(x,y,\nu)$ is the Schwartz kernel of spectral projector for potential W, approximating W^{TF} and $\nu\le 0$ is a chemical potential. One can prove easily that $\|\rho_F\|_{5/3}^{5/3}$ satisfies the same estimate and we need to estimate $\operatorname{Tr}\bigl(\gamma_\Psi(I-E(\mu))\bigr)$.

Consider

$$\begin{aligned}
&N\langle H_{A,W(x_1)}\Psi,\Psi\rangle-\operatorname{Tr}(HE(\nu))-\alpha\operatorname{Tr}\bigl(\gamma_\Psi(I-E(\nu))\bigr)\\
&\qquad\ge\int_{\beta<0}\beta\, d_\beta \operatorname{Tr}E(\beta)-\int_{\beta\le\nu}(\beta-\nu+\alpha)\,d_\beta\operatorname{Tr}E(\beta)\\
&\qquad=-\int_{\nu-\alpha<\beta<\nu}(\beta-\nu+\alpha)d_\beta E(\beta)\\
&\qquad=-\alpha E(\nu)+\int_{\nu-\alpha<\beta<\nu}E(\beta)\,d\beta.
\end{aligned}\tag{26.A.21}$$

We can replace $E(\beta)$ by $\int P'(W+\beta)\,dx$ with a resulting error $O(Z\alpha\hbar^\delta)$, $\hbar:=BZ^{-3}$. Then the right-hand expression becomes

$$\begin{aligned}
-L(\alpha)&:=\int\Bigl(-\alpha P'_B(W+\nu)+\int_0^\alpha P'_B(W+\nu-\beta)\,d\beta\Bigr)\,dx=\\
&\qquad-\int_0^\alpha(\alpha-\beta)\Bigl(\int P''_B(W+\nu-\beta)\,dx\Bigr)\,d\beta.
\end{aligned}\tag{26.A.22}$$

Therefore

$$\begin{aligned}
&\alpha\Bigl(\operatorname{Tr}\bigl(\gamma_\Psi(I-E(\mu))\bigr)-CZ\hbar^\delta\Bigr)\le\\
&\qquad\underbrace{N\langle H_{A,W(x_1)}\Psi,\Psi\rangle-\operatorname{Tr}(HE(\nu))}+L(\alpha).
\end{aligned}\tag{26.A.23}$$

Note that adding to the selected terms $-\frac{1}{2}\mathsf{D}(\rho^{\mathsf{TF}},\rho^{\mathsf{TF}})$ we obtain exactly the snippet, occurring in the lower estimate of E_N, but in virtue of the upper estimate it should not exceed $Q = CZ^{\frac{5}{3}}\bigl(1 + BZ^{-\frac{4}{3}}\bigr)^{\frac{2}{5}} \le CZ^{\frac{5}{3}} + Ch^2Z^{\frac{7}{3}}$, and therefore, plugging $\alpha = Z^{\frac{4}{3}}\hbar^{\delta}$, we conclude that

$$\operatorname{Tr}\bigl(\gamma_\Psi(I - E(\mu)\bigr) \le Z\hbar^{\delta} \tag{26.A.24}$$

provided we prove that

$$L(\alpha) \le Q \qquad \text{for}\ \ \alpha = Z^{\frac{4}{3}}\hbar^{\delta}. \tag{26.A.25}$$

Therefore modulo proof of (26.A.25) we arrive to the estimate (26.A.26) below:

Theorem 26.A.3. *Let $N \asymp Z$ and $B \le Z$. Then for the ground state energy*

$$\sum_{1\le j<k\le N} \int |x_j - x_k|^{-1}|\Psi(x_1, \dots, x_N)|^2\, dx_1\cdots dx_N \ge \\ \frac{1}{2}\mathsf{D}(\rho^{\mathsf{TF}}, \rho^{\mathsf{TF}}) + \mathsf{Dirac} - CZ^{\frac{5}{3}-\delta}(1 + B^{\delta}) \tag{26.A.26}$$

To prove (26.A.25) we note that $0 \le P''_B(w) \asymp w^{\frac{1}{2}} + Bw^{-\frac{1}{2}}$. One can prove easily then that $L(\alpha) \le C\alpha^{\frac{7}{4}} + CB^{\frac{1}{4}}\alpha^{\frac{3}{2}}$, which obviously implies (26.A.25).

26.A.2 Very Strong Magnetic Field Case

Let us consider now case $Z^2 \le B \le Z^3$.

Proposition 26.A.4. *Consider the Schrödinger operator $H_{A,W}$ with a constant magnetic field of intensity B and potential W: $W \le Z|x|^{-1}$. Let $\phi(x) := \phi_r(x)$ be r-admissible function. Then if $Z^2 \lesssim B \lesssim Z^3$ and $r \asymp Z^{-1}$*

$$|e(x, y, 0)| \le CZB \qquad \textit{in}\ \ B(0, r) \tag{26.A.27}$$

and

(26.A.28) *All eigenvalues are $\ge -CZ^2$.*

Proof. Without any loss of the generality one can assume that

$$H_{A,W} = D_3^2 + D_2^2 + (D_1 - Bx_2)^2 - W. \tag{26.A.29}$$

Consider $f \in \mathscr{L}^2$; then $\|E(\lambda)f\| \le \|f\|$ and then one can prove easily (26.A.28) and inequality

$$\|H_{A,0}E(\lambda)f\| \le (CZ^2+\lambda_+)\|f\|. \tag{26.A.30}$$

Indeed, $\frac{1}{2}D_3^2 + CZ^2 \ge W$ in the operator sense.

Then (26.A.30) implies that in $B(0,r)\times B(y',r')$ with $r'=B^{-\frac{1}{2}}$

$$|P^\alpha E(\lambda)f| \le CZ^{\alpha_3}B^{\frac{1}{2}|\alpha'|} \qquad \forall \alpha : |\alpha|\le 2\ \forall \lambda \le Z^2$$

with $P=(D_1-Bx_2, D_2, D_3)$ and therefore $\|E(\lambda)f\|_{\mathscr{C}} \le CZ^{\frac{1}{2}}B^{\frac{1}{2}}\|f\|$. Then $\|E(x,.,\lambda)\|_{\mathscr{L}^2_y}\| \le CZ^{\frac{1}{2}}B^{\frac{1}{2}}$.

Repeating the same arguments with respect to y we arrive to estimate (26.A.27). □

The following corollary follows immediately:

Corollary 26.A.5. *In the framework of Proposition 26.A.4 with* $\phi \in \mathscr{L}^\infty(B(0,r))$, $\|\phi\|_{\mathscr{L}^\infty}\le 1$

$$|\int \phi(x)e(x,x,0)\,dx| \le CZ^{-2}B, \tag{26.A.31}$$

$$\mathsf{D}\bigl(\phi(x)e(x,x,0),\phi(x)e(x,x,0)\bigr) \le CZ^{-3}B^2 \tag{26.A.32}$$

and

$$|\int_{-\infty}^0 \int \phi(x)e(x,x,\tau)\,d\tau dx| \le CB. \tag{26.A.33}$$

26.A.3 Riemann Sums and Integrals

If $f\in\mathscr{C}^\infty(\mathbb{R}^+)$ and fast decays at $+\infty$, then

$$f(0)h+\sum_{n\ge1}2f(2nh)h \sim \int_0^\infty f(t)\,dt + \sum_{m\ge1}\kappa_m f^{(2m-1)}(0)h^{2m}, \tag{26.A.34}$$

$$\sum_{n\ge0}2f((2n+1)h)h \sim \int_0^\infty f(t)\,dt + \sum_{m\ge1}\kappa'_m f^{(2m-1)}(0)h^{2m} \tag{26.A.35}$$

as $h\to+0$. The proofs of both formulae follow from the Taylor's decomposition and observation that the odd powers of h should disappear. Taking

$f(t)=e^{-tz/h}$ with $\operatorname{Re} z>0$ we arrive to

$$1-\frac{\cosh(z)}{\sinh(z)}z \sim \sum_{m\ge 1}\kappa_m z^{2m}, \tag{26.A.36}$$

$$1-\frac{1}{\sinh(z)}z \sim \sum_{m\ge 1}\kappa'_m z^{2m} \tag{26.A.37}$$

for $|z|\ll 1$. In particular, $\kappa_1=\frac{1}{3}$ and $\kappa'_1=-\frac{1}{6}$.

26.A.4 Some Spectral Function Estimates

Proposition 26.A.6. *For the Schrödinger operator with $A, W\in \mathscr{C}^\infty$ and for $\phi\in\mathscr{C}_0^\infty([-1,1])$ the following estimate holds for any s:*

$$|F(x,y)|\le C(\mu h+1)h^{-3}\bigl(1+h^{-1}|x-y|\bigr)^{-s} \tag{26.A.38}$$

where

$$F(x,y):=\int \phi(\lambda)\, d_\lambda e(x,y,\lambda). \tag{26.A.39}$$

Proof. Let $u(x,y,t)=\int e^{-ih^{-1}t\lambda}\,d_\lambda e(x,y,\lambda)$ be the Schwartz's kernel of $e^{-ih^{-1}Ht}$.

Let us fix y. Note first that $\mathscr{L}^2$-norm[52] of $\phi(hD_t)\chi(t)\omega(x)u(x,y,t)$ is less than Ch^s for $\chi\in\mathscr{C}_0^\infty([-\epsilon,\epsilon])$ and $\omega\in\mathscr{C}^\infty$ supported in $\{x\colon |x-y|\ge \epsilon_1\}$ (with $\epsilon_1=C\epsilon$) due to the finite speed of propagation of singularities.

We conclude then that $\mathscr{L}^2$-norm of $\phi(hD_t)\chi(t)\omega(x)u(x,y,t)$ does not exceed $C(\mu h+1)h^s$ for $\omega\in\mathscr{C}^\infty$ supported in $\{x\colon |x-y|\ge C\}$.

Then $\mathscr{L}^2$-norm of $\partial_t^l\nabla^\alpha\phi(hD_t)\chi(t)\omega(x)u$ does not exceed $C(\mu h+1)h^s$. Therefore due to imbedding inequality $\mathscr{L}^\infty$-norm of $\phi(hD_t)\chi(t)\omega(x)u$ also does not exceed $C(\mu h+1)h^s$. Setting $t=0$ and using this inequality and estimate $|F(x,y)|\le C(\mu h+1)h^{-3}$ (due to Chapter 7), we conclude that $|F(x,y)|\le C(\mu h+1)h^s$ for $|x-y|\ge\epsilon_0$.

Now let us consider general x with $|x-y|=r\ge Ch$. Then rescaling $(x-y)\mapsto(x-y)r^{-1}$ we need also to rescale $h\mapsto hr^{-1}$, $\mu\mapsto\mu r$ and rescaling the above inequality and keeping in mind that $F(x,y)$ is a density with respect to x, we conclude that $|F(x,y)|\le Ch^s r^{-3-s}$ which is equivalent to (26.A.38)–(26.A.39). □

[52] With respect to x,t here and below.

26.A.5 Zhislin's Theorem for Constant Magnetic Field

We provide just a scheme to prove Zhislin's theorem in the case of the constant magnetic field. In this analysis $\underline{Z}$, $\underline{y}$, N and B are constant.

Proposition 26.A.7. *Let* $\Psi = \Psi_N$ *be the ground state with the energy* $\mathsf{E}_N < \mathsf{E}_{N-1}$. *Then*

(i) $\Psi \in \mathscr{C}^1$ *and* $\Psi = O(e^{-\epsilon|\underline{x}|})$ *as* $|\underline{x}| \to \infty$.

(ii) Let $N < Z$. *Then* $V_\Psi - V \in \mathscr{C}^2$ *and* $V_\Psi = (Z-N)|x|^{-1} + O(|x|^{-2})$, $\nabla V_\Psi = (Z-N)|x|^{-2} + O(|x|^{-3})$ *as* $|x| \to \infty$.

Proof. Obvious proof is left to the reader. □

Theorem 26.A.8 (Zhislin's theorem). $\mathsf{E}_{N+1} < \mathsf{E}_N$ *for* $N < Z$.

Proof. We can assume that $\mathsf{E}_N < 0$ and the ground state energy exists. Really, it is true for some $N < Z$ and if we prove that then automatically $\mathsf{E}_{N+1} < \mathsf{E}_N$, then it would be true for $(N+1)$ as well, so we may go by induction.

Consider $\Psi = \Psi_N(x_1, \dots, x_N)$ and also $\tilde{\Psi}_{N+1}$, which is an antisymmetrized $\Psi_N(x_1, \dots, x_N)u(x_{N+1})$ (cf. (26.8.21)):

$$\tilde{\Psi} = \tilde{\Psi}(x_1, \dots, x_{N+1}) = \Psi(x_1, \dots, x_N)u(x_{n+1}) - \sum_{1\le j\le N} \Psi(x_1, \dots, x_{j-1}, x_{N+1}, x_{j+1}, \dots, x_N)u(x_j). \tag{26.A.40}$$

Then like in the estimate of the ionization energy (cf. (26.8.22)–(26.8.23)):

$$N^{-1}\mathsf{I}_{N+1}\|\tilde{\Psi}\|^2 \ge -\langle H_{V,x_{N+1}}\Psi u, \tilde{\Psi}\rangle - \langle \sum_{1\le i\le N} |x_i - x_{N+1}|^{-1}\Psi u, \tilde{\Psi}\rangle \tag{26.A.41}$$

and

$$N^{-1}\|\tilde{\Psi}\|^2 = \|\Psi\|^2 \cdot \|u\|^2 - N\int \Psi(x_1, \dots, x_{N-1}, x)\Psi^\dagger(x_1, \dots, x_{N-1}, y)u(y)u^\dagger(x)\, dx_1 \cdots dx_{N-1}\, dxdy. \tag{26.A.42}$$

Now let us consider u supported in $\{x\colon \frac{1}{2}a \le |x| \le 3a\}$ with a to be chosen later. Then in virtue of Proposition 26.A.7(i) modulo $O(e^{-\epsilon_1 a})$ we can replace in the right-hand expressions $\tilde{\Psi}$ by $\Psi_N(x_1,\ldots,x_N)u(x_{N+1})$ resulting in $-\langle H_W u, u\rangle$ and $\|u\|^2$ respectively with $W = V_\Psi$ defined in Proposition 26.A.7(ii).

Therefore all we need to prove this theorem is to be able to select u with $\|u\| \asymp 1$, supported in $\{x\colon a \le |x| \le 3a\}$ and with $\langle H_W u, u\rangle \le -\epsilon_0 a^{-1}$.

In virtue of Proposition 26.A.7(ii) $V_\Psi \ge \epsilon_0 a^{-1}$ in $\{x\colon a \le |x| \le 3a\}$ and therefore we can replace W by $\epsilon_0 a^{-1}$. Without any loss of the generality one can assume that $A = (Bx_2, 0, 0)$. Recall that for the linear vector-potential $\vec{A}$ operator $H_0 = ((i\nabla - A)\cdot \boldsymbol{\sigma})^2$ is a direct sum of $H_0^+ = (i\nabla - A)^2 + B$ and $H_0^- = (i\nabla - A)^2 - B$; so we can consider only the latter. Note that $H_0^- = (i\partial_1 - Bx_2)^2 - \partial_2^2 - \partial_3^2$ and $H_0^- v = 0$ with $v = \exp(-\frac{1}{2}B(x_2 - a)^2 + iBax_1)$.

Then $u = v(x)\chi(r^{-1}(x - \bar{x}))$ with $\chi \in \mathscr{C}^\infty(B(0,1))$, $\chi = 1$ in $B(0,\frac{1}{2})$, $\bar{x} = (0, 2a, 0)$, $r = \frac{1}{3}a$ is a required function. □

Comments

We already mentioned papers E. H. Lieb, J. P. Solovej and J. Yngvason [1,3] where asymptotics of the ground state energy were derived in the cases $B \ll Z^3$ and $B \gg Z^3$ respectively. Intermediate case $B \sim Z^3$ was covered also in [1]. Even without remainder estimates certain results concerning ionization energy and maximal possible positive and negative charges were also derived.

Remainder estimates in the case $B \ll Z^3$ were derived by V. Ivrii in [20, 21]. Unfortunately there are gaps in the proofs of the second paper in the case of $M \ge 2$ and large $Z - N > 0$ which I was unable to fill.; so our results in this case are not as sharp as they supposed to be.

Chapter 27

The Case of Self-Generated Magnetic Field

27.1 Introduction

We are going to replace Schrödinger operator without magnetic field as in Chapter 25 or with a constant magnetic field as in Chapter 26 by Schrödinger operator

$$H = H_{A,V} = \bigl((D - A)\cdot \boldsymbol{\sigma}\bigr)^2 - V(x) \tag{27.1.1}$$

with unknown magnetic field A but then to add to the ground state energy of the atom (or molecule) the energy of magnetic field (see selected term in (27.1.2) thus arriving to

$$\mathsf{E}(A) = \inf \operatorname{Spec}(\mathsf{H}_{A,V}) + \underbrace{\alpha^{-1}\int |\nabla \times A|^2\,dx} \tag{27.1.2}$$

with N-particle quantum Hamiltonian $\mathsf{H}_{A,V}$ defined by (26.1.1) and a parameter $\alpha \in (0, \kappa^* Z^{-1}]$ with small constant $\kappa^* > 0$.

Then finally

$$\mathsf{E}^* = \inf_{A\in \mathscr{H}^1_0} \mathsf{E}(A) \tag{27.1.3}$$

defines a ground state energy with a *self-generated magnetic field*[1)].

[1)] This notion was introduced in series of papers L. Erdös, S. Fournais and J. P. Solovej [1,3,4]; see also L. Erdös and J. P. Solovej [1].

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First of all we are lacking so far a semiclassical local theory and we are developing it in Section 27.2 where we consider one-particle quantum Hamiltonian

$$H = H_{A,V} = \bigl((hD - A)\cdot \boldsymbol{\sigma}\bigr)^2 - V(x) \tag{27.1.4}$$

but instead of $\inf \operatorname{Spec}(\mathsf{H}_{A,V})$ we consider $\operatorname{Tr}^-(H_{A,V})$ which as we already know is what replaces $\inf \operatorname{Spec}(\mathsf{H}_{A,V})$ if electrons do not interact (then if electrons interact we will need to replace V by W which includes a potential generated by the electron cloud and justify this by estimating an error).

We define the energy of the magnetic field as in (27.1.2) but with κ replaced by κh^{d-1} (here $d \ge 2$ is arbitrary) and we prove that for $d = 2, 3$ in this framework a self-generated magnetic field is weak and the asymptotics with the remainder $O(h^{2-d})$ (or even $o(h^{2-d})$ under standard assumption of the global nature) is exactly as for $\kappa = 0$ (i.e. with $A = 0$). In the latter case asymptotics includes the Schwinger correction term $\varkappa_2 h^{-1}$.

Then in Section 27.3 we consider operator with potential having Coulomb-type singularities and combining results and arguments of Sections 27.2 and 12.6 prove for $d = 3$ that

$$\operatorname{Tr}^-(H_{A,V}) = \mathsf{Weyl}_1 + 2S(\kappa)h^{-2} + O\bigl(\kappa|\log\kappa|^{\frac{1}{3}} h^{-\frac{4}{3}} + h^{-1}\bigr) \tag{27.1.5}$$

provided $\kappa < \kappa^*$ (which is a small constant) and there is just one singularity; when there are several singularities with a minimal distance $a \gg 1$ between them we prove that

$$\operatorname{Tr}^-(H_{A,V}) = \mathsf{Weyl}_1 + 2S(\kappa)h^{-2} + O\bigl(\kappa|\log\kappa|^{\frac{1}{3}} h^{-\frac{4}{3}} + h^{-1} + \kappa a^{-3}h^{-2}\bigr). \tag{27.1.6}$$

If $\kappa \ll h^{\frac{1}{3}}|\log h|^{-\frac{1}{3}}$ then under standard assumption about trajectories we can upgrade this asymptotics to even sharper with the remainder estimate $o(h^{-1})$ and with the Schwinger correction term.

Further, in Section 27.4 we apply these results to provide estimates from above and below for the total energy (27.1.3). As a byproduct we also estimate $\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}},\, \rho_\Psi - \rho^{\mathsf{TF}})$ where Ψ is a ground state for a near-minimizer A.

This estimate enables us in Section 27.5 to derive upper estimates for the excessive negative charge, estimates or asymptotics for the ionization energy, and in the free nuclei model also for the minimal distance between nuclei and (in the case of molecule) for the excessive positive charge.

27.2 Local Semiclassical Trace Asymptotics

27.2.1 Toy-Model

Statement of the Problem

Let us consider operator (27.1.1) in $\mathbb{R}^d$ with $d=3$ where A, V are real-valued functions and $V \in \mathscr{L}^{\frac{5}{2}} \cap \mathscr{L}^4$, $A \in \mathscr{H}^1_0$. Then this operator is self-adjoint. We are interested in $\mathsf{Tr}^-(H_{A,V})$ (the sum of all negative eigenvalues of this operator). Let

$$\mathsf{E}^* := \inf_{A\in\mathscr{H}^1_0(B(0,r))} \mathsf{E}(A), \tag{27.2.1}$$

$$\mathsf{E}(A) := \Bigl(\mathsf{Tr}^- H_{A,V} + \kappa^{-1}h^{-2}\int |\partial A|^2\, dx\Bigr) \tag{27.2.2}$$

with $\partial A = (\partial_i A_j)$ a matrix; here and below r is a parameter and constants do not depend on it.

The estimate from above is delivered by $A=0$ and Weyl formula with an error $O(h^{-1})$ as $V\in\mathscr{C}^{2,1}$ [2)]

$$\mathsf{E}^* \le \mathsf{Weyl}_1 + O(h^{-1}); \tag{27.2.3}$$

where

$$\mathsf{Weyl}(\tau) = \frac{1}{3\pi^2}h^{-3}\int (V+\tau)_+^{\frac{3}{2}}\, dx, \tag{27.2.4}$$

and

$$\mathsf{Weyl}_1 = \int_{-\infty}^0 \tau \mathsf{d}_\tau \mathsf{Weyl}(\tau) = -\frac{2}{15\pi^2}\int V_+^{\frac{5}{2}}\, dx. \tag{27.2.5}$$

Also for estimates $o(h^{-2})$ we need to include into Weyl_1 the corresponding boundary term. Now our goal is to provide an estimate from below

$$\mathsf{E}^* \ge \mathsf{Weyl}_1 - O(h^{-1}); \tag{27.2.6}$$

We will use also $\mathsf{Weyl}(x,\tau)$ and $\mathsf{Weyl}_1(x)$ defined the same way albeit without integration with respect to x.

[2)] Recall that this means that the second derivatives of V are continuous with the continuity modulus $O(|\log|x-y||^{-1})$, see Section 4.6. If there is a boundary it does not pose any problem provided it is in the classically forbidden region.

Preliminary Analysis

So, let us estimate $\mathsf{E}(A)$ from below. First we need the following really simple

Proposition 27.2.1. *Let $V \in \mathscr{L}^{\frac{5}{2}} \cap \mathscr{L}^4$. Then*

$$\mathsf{E}^* \ge -Ch^{-3} \tag{27.2.7}$$

and either

$$\frac{1}{\kappa h^2}\int |\partial A|^2\,dx \le Ch^{-3} \tag{27.2.8}$$

or $\mathsf{E}(A) \ge ch^{-3}$.

Proof. Using the Magnetic Lieb–Thirring inequality (5) of E. H. Lieb, M. Loss, M. and J. P. Solovej [1])

$$\int \operatorname{tr} e_1(x,x,\tau)\,dx \ge \\ -Ch^{-3}\int V_+^{\frac{5}{2}}\,dx - Ch^2\Bigl(h^{-2}\int |\partial A|^2\,dx\Bigr)^{\frac{3}{4}}\Bigl(h^{-8}\int V_+^4\,dx\Bigr)^{\frac{1}{4}}, \tag{27.2.9}$$

we conclude that for any $\delta > 0$

$$\mathsf{E}(A) \ge -Ch^{-3} - C\delta^3 h^{-3} + \bigl(\kappa^{-1}h^{-2} - \delta^{-1}h^{-1}\bigr)\int |\partial A|^2\,dx \tag{27.2.10}$$

which implies both assertions of this proposition. □

Proposition 27.2.2. *Let $V_+ \in \mathscr{L}^{\frac{5}{2}} \cap \mathscr{L}^4$, $\kappa \le ch^{-1}$ and*

$$V \le -C^{-1}(1+|x|)^{\delta} + C. \tag{27.2.11}$$

Then there exists a minimizer A.

Proof. Consider a minimizing sequence A_j. Without any loss of the generality one can assume that $A_j \to A_\infty$ weakly in $\mathscr{H}^1$ and in $\mathscr{L}^6$ and strongly in $\mathscr{L}^p_{\mathsf{loc}}$ with any $p < 6$ [3)]. Then A_∞ is a minimizer.

Really, due to (27.2.8) and (7.2.11) negative spectra of $H_{A_j,V}$ are discrete and the number of negative eigenvalues is bounded by $N = N(h)$. Consider

[3)] Otherwise we select a converging subsequence.

ordered eigenvalues $\lambda_{j,k}$ of $H_{A_j,V}$. Without any loss of the generality one can assume that $\lambda_{j,k}$ have limits $\lambda_{\infty,k} \le 0$ (we go to the subsequence if needed).

We claim that $\lambda_{\infty,k}$ are also eigenvalues and if $\lambda_{\infty,k} = \ldots = \lambda_{\infty,k+r-1}$ then it is eigenvalue of at least multiplicity r. Indeed, let $u_{j,k}$ be corresponding eigenfunctions, orthonormal in $\mathscr{L}^2$. Then in virtue of A_j being bounded in $\mathscr{L}^6$ and $V \in \mathscr{L}^4$ we can estimate

$$\|Du_{j,k}\| \le K\|u_{j,k}\|_6^{1-\sigma} \cdot \|u_{j,k}\|^\sigma \le K\|Du_{j,k}\|^{1-\sigma} \cdot \|u_{j,k}\|^\sigma$$

with $\sigma > 0$ which implies $\|Du_{j,k}\| \le K$. Also assumption (27.2.11) implies that $\|(1+|x|)^{\delta/2}u_{j,k}\|$ are bounded and therefore without any loss of the generality one can assume that $u_{j,k}$ converge strongly.

Then

$$\lim_{j\to\infty} \operatorname{Tr}^-(H_{A_j,V}) \ge \operatorname{Tr}^-(H_{A_\infty,V}), \tag{27.2.12}$$

$$\liminf_{j\to\infty} \int |\partial A_j|^2\,dx \ge \int |\partial A_\infty|^2\,dx \tag{27.2.13}$$

and therefore $\mathsf{E}(A_\infty) \le \mathsf{E}^*$. Then A_∞ is a minimizer and there are equalities in (27.2.12)–(27.2.13) and, in particular, there no negative eigenvalues of $H_{A_\infty,V}$ other than $\lambda_{\infty,k}$. □

Remark 27.2.3. We do not know if a minimizer is unique. Also we do not impose here any restrictions on r, K (which may depend on h) in (27.2.11) or $\kappa > 0$. From now on until the further notice let $A = A_h$ be a minimizer.

Proposition 27.2.4. *In the framework of Proposition 27.2.2 let A be a minimizer. Then*

$$\frac{2}{\kappa h^2}\Delta A_j(x) = \Phi_j := \\ -\operatorname{Re}\operatorname{tr}\Bigl[\upsigma_j\Bigl((hD-A)_x\cdot\boldsymbol{\upsigma} e(x,y,\tau) + e(x,y,\tau)\,{}^t(hD-A)_y\cdot\boldsymbol{\upsigma}\Bigr)\Bigr]\Bigr|_{y=x} \tag{27.2.14}$$

where $A = (A_1, A_2, A_3)$, $\boldsymbol{\upsigma} = (\upsigma_1, \upsigma_2, \upsigma_3)$ and $e(x, y, \tau)$ is the Schwartz kernel of the spectral projector $\uptheta(-H)$ of $H = H_{A,V}$ and tr is a matrix trace.

Proof. Consider variation δA of A and variation of $\operatorname{Tr}^-(H) = \operatorname{Tr}(H^-)$ where $H^- = H\uptheta(-H)$ is a negative part of H. Note that the spectral projector of H is

$$\uptheta(\tau - H) = \frac{1}{2\pi i}\int_{-\infty}^{\tau} \operatorname{Res}_{\mathbb{R}}(\tau - H)^{-1} \tag{27.2.15}$$

and therefore

$$\delta \operatorname{Tr}\bigl(\theta(\tau-H)\bigr)=\frac{1}{2\pi i}\int_{-\infty}^{\tau}\operatorname{Res}_{\mathbb{R}}\operatorname{Tr}\bigl((\tau-H)^{-1}(\delta H)(\tau-H)^{-1}\bigr)=\\
\frac{1}{2\pi i}\int_{-\infty}^{\tau}\operatorname{Res}_{\mathbb{R}}\operatorname{Tr}\bigl((\delta H)(\tau-H)^{-2}\bigr)=-\partial_\tau\frac{1}{2\pi i}\int_{-\infty}^{\tau}\operatorname{Res}_{\mathbb{R}}\operatorname{Tr}\bigl((\delta H)(\tau-H)^{-1}\bigr)=\\
-\partial_\tau\operatorname{Tr}\bigl((\delta H)\theta(\tau-H)\bigr).$$

Plugging it into

$$\operatorname{Tr}^-(H)=\int_{-\infty}^{0}\tau d_\tau \operatorname{Tr}\bigl(\theta(\tau-H)\bigr)=-\int_{-\infty}^{0}\operatorname{Tr}\bigl(\theta(\tau-H)\,d\tau\bigr)\tag{27.2.16}$$

and integrating with respect to τ we arrive after simple calculations to

$$\delta\operatorname{Tr}^-(H-\tau)=\operatorname{Tr}\bigl((\delta H)\theta(\tau-H)\bigr)=\sum_j\int\Phi_j(x)\delta A_j(x)\,dx\tag{27.2.17}$$

where $\Phi(x)$ is the right-hand expression of (27.2.14). Therefore

$$\delta\mathsf{E}(A)=\sum_j\int\bigl(\Phi_j(x)-\frac{2}{\kappa h^2}\Delta A_j(x)\bigr)\delta A_j(x)\,dx\tag{27.2.18}$$

which implies (27.2.14). □

Proposition 27.2.5. *If for $\kappa=\kappa^*$*

$$\mathsf{E}^*\ge \mathsf{Weyl}_1-CM\tag{27.2.19}$$

with $M\ge Ch^{-1}$ then for $\kappa\le\kappa^*(1-\epsilon_0)$

$$\frac{1}{\kappa h^2}\int|\partial A|^2\,dx\le C_1M.\tag{27.2.20}$$

Proof. Proof is obvious based also on the upper estimate $\mathsf{E}^*\le\mathsf{Weyl}_1+Ch^{-1}$. □

Estimates

Proposition 27.2.6. *Let estimate* (27.2.20) *be fulfilled and let*

$$\varsigma = \kappa M h \le c. \tag{27.2.21}$$

Then for $\tau \le c$

(i) Operator norm in $\mathscr{L}^2$ *of* $(hD)^k \theta(\tau - H)$ *does not exceed* C *for* $k = 0, 1, 2$.

(ii) Operator norm in $\mathscr{L}^2$ *of* $(hD)^k \bigl((hD - A)\cdot \boldsymbol{\sigma}\bigr)\theta(\tau - H)$ *does not exceed* C *for* $k = 0, 1$.

Proof. (i) Let $u = \theta(\tau - H)f$. Then $\|u\| \le \|f\|$ and since

$$\|A\|_{\mathscr{L}^6} \le C\|\partial A\| \le C(\kappa M)^{\frac{1}{2}} h \tag{27.2.22}$$

we conclude that

$$\begin{gathered}
\|hDu\| \le \|(hD - A)u\| + \|Au\| \le \|(hD - A)u\| + C\|A\|_{\mathscr{L}^6}\cdot \|u\|_{\mathscr{L}^3} \le \\
\|(hD - A)u\| + C(\kappa M)^{\frac{1}{2}} h\|u\|^{1/2}\cdot \|u\|^{1/2}_{\mathscr{L}^6} \le \\
\|(hD - A)u\| + C(\kappa Mh)^{\frac{1}{2}}\|u\|^{1/2}\cdot \|hDu\|^{1/2} \le \\
\|(hD - A)u\| + \frac{1}{2}\|hDu\| + C\kappa Mh\|u\|;
\end{gathered}$$

therefore due to (27.2.21)

$$\|hDu\| \le 2\|(hD - A)u\| + C\kappa Mh\|u\|. \tag{27.2.23}$$

On the other hand, for $B = \nabla \times A$ and $\tau \le c$

$$\begin{gathered}
\|(hD - A)u\|^2 \le C\|u\|^2 + (h|B|u, u) \le C\|u\|^2 + h\|B\|\cdot \|u\|^2_{\mathscr{L}^4} \le \\
C\|u\|^2 + C(\kappa M)^{\frac{1}{2}} h^2\|u\|\cdot \|u\|_{\mathscr{L}^6} \le C\|u\|^2 + C(\kappa M)^{\frac{1}{2}} h\|u\|\cdot \|hDu\| \le \\
C(1 + \kappa Mh^2 + \kappa^{\frac{3}{2}} M^{\frac{3}{2}} h^2)\|u\|^2 + \frac{1}{2}\|(hD - A)u\|^2
\end{gathered}$$

and due to (27.2.23) we conclude that

$$\|(hD - A)u\| \le C\|u\| \quad \text{and} \quad \|hDu\| \le C(1 + \kappa Mh)\|u\| \tag{27.2.24}$$

provided $\kappa M h^{1+\delta}\le c$ for sufficiently small $\delta>0$. Therefore under assumption (27.2.21) for $k=0,1$ statement (i) is proven.

Further, since $(hD)^2=(hD-A)^2+A(hD-A)+AhD-h[D,A]$ we in the same way as before (and using (27.2.24)) conclude that

$$\|(hD)^2u\|\le C\|u\|^2+\frac{1}{4}\|hD(hD-A)u\|+\frac{1}{4}\|h^2D^2u\|$$

and therefore

$$\|h^2D^2u\|\le C\|u\|^2+C\|AhDu\|$$

and repeating the same arguments we get $\|h^2D^2u\|\le C\|u\|$; so for $k=2$ Statement (i) is also proven.

(ii) Statement (ii) is proven in the same way. □

Corollary 27.2.7. *Let* (27.2.20) *and* (27.2.21) *be fulfilled. Then for* $\tau\le c$

(27.2.25) $$e(x,x,\tau)\le Ch^{-3}$$

and

(27.2.26) $$|((hD-A)\cdot\boldsymbol{\sigma})e(x,y,\tau)|_{x=y}|\le Ch^{-3}.$$

Proof. Let us prove that

(27.2.27) Operator norms from $\mathscr{L}^2$ to $\mathscr{C}$ of both operators $\theta(\tau-H)$ and $((hD-A)\cdot\boldsymbol{\sigma})\theta(\tau-H)$ do not exceed $Ch^{-\frac{3}{2}}$.

Indeed, Proposition 27.2.6 and embedding theorem imply that the operator norm of $\theta(\tau-H)$ from $\mathscr{L}^2$ to C does not exceed $Ch^{-\frac{3}{2}}$. Then due to interpolation operator norms of $\theta(\tau-H)$ from $\mathscr{L}^2$ to $\mathscr{L}^3$ and $\mathscr{L}^6$ do not exceed $Ch^{-\frac{1}{2}}$ and Ch^{-1} respectively.

Let $v=((hD-A)\cdot\boldsymbol{\sigma})u$, $u=\theta(\tau-H)f$, $\|f\|=1$. We know that $\mathscr{L}^6$-norms of Hu and u do not exceed Ch^{-1}, and then it is true for $((hD-A)\cdot\boldsymbol{\sigma})u\|$ as well.

Then $\|Au\|_{\mathscr{L}^3} \le C\|A\|_{\mathscr{L}^6}\|f\|_{\mathscr{L}^6} \le Ch^{-\frac{1}{2}}$ and $\|Du\|_{\mathscr{L}^3} \le Ch^{-\frac{3}{2}}$ which together with $\|u\|_{\mathscr{L}^2} \le C$ implies that $\|u\|_{\mathscr{L}^p} \le Ch^{-3/2+3/p}$ for $2 \le p < \infty$. Then $\|Au\|_{\mathscr{L}^4} \le C\|A\|_{\mathscr{L}^6}\|u\|_{\mathscr{L}^{12}} \le Ch^{-\frac{1}{4}}$ and $\|Du\|_{\mathscr{L}^4} \le Ch^{-\frac{5}{4}}$. Together with $\|u\| \le C$ it implies $\|u\| \le Ch^{-\frac{3}{2}}$. So, (27.2.27) has been proven.

Then the same estimate for holds adjoint operators which imply both statements of the corollary. □

Corollary 27.2.8. *Let* (27.2.20) *and* (27.2.21) *be fulfilled and A be a minimizer. Then*

$$\|\partial A\|_{\mathscr{C}^{1-\delta}} \le C\kappa h^{-1} \tag{27.2.28}$$

and

$$\|\partial A\|_{\mathscr{L}^\infty} \le C'_\delta h^{-\frac{4}{5}-\delta} \tag{27.2.29}$$

where $\mathscr{C}^\theta$ is the scale of Hölder spaces and $\delta > 0$ is arbitrarily small.

Proof. Really, due to (27.2.14) minimizer A satisfies $\|\Delta A\|_{\mathscr{L}^\infty} \le C\kappa h^{-1}$. Also we know that $\|\partial A\| \le C(\kappa M h^2)^{\frac{1}{2}} \le Ch^{\frac{1}{2}}$ due to (27.2.21). Then (27.2.28) holds due to the standard properties of the elliptic equations[4)].

Therefore if at some point y we have $|\partial A(y)| \gtrsim \mu$, it is true in its $\epsilon(\mu h\kappa^{-1})^{1-\delta}$-vicinity (provided $\mu \le \kappa h^{-1}$) and then

$$\|\partial A\|^2 \gtrsim \mu^2(\mu h\kappa^{-1})^{3(1-\delta)}$$

and we conclude that

$$\mu^2(\mu h\kappa^{-1})^{3(1-\delta)} \le C\kappa h^2 M \iff \mu^{5-3\delta} \le C\kappa^{4-3\delta}h^{-1+3\delta}M$$

and one can see easily that (27.2.29) holds due to (27.2.21) and assumption $h^{-1} \le M \lesssim h^{-3}$.

On the other hand, if $\mu \ge \kappa h^{-1}$ then we need to take ϵ-vicinity and then $\mu^2 \le C\kappa M h^2 \le Ch^{\frac{1}{2}}$ where we used (27.2.21) again. Therefore (27.2.29) has been proven. □

Remark 27.2.9. (i) It is not clear if it is possible to generalize this theory to arbitrary $d \ge 2$ with the magnetic field energy given by

$$\frac{1}{\kappa h^{d-1}}\int \bigl(|\partial A|^2 - |\nabla \cdot A|^2\bigr)\,dx. \tag{27.2.30}$$

4) Actually we can slightly improve this statement.

Surely one should use generalized Pauli matrices σ_j in the definition of the operator: for $d=2$ one can prove that $\mathsf{E}(A)$ is bounded from below and a minimizer exists; for $d=4$ one can prove that $\mathsf{E}(A)$ is bounded from below if $\kappa \le \epsilon_0 h$; especially problematic is the case $d\ge 5$ since then $A\in \mathscr{H}^1$ does not guarantee enough regularity.

(ii) Therefore while arguments of Subsection 27.2.2 below remain valid for $d\ge 4$, so far they remain conditional (if a minimizer exists and satisfies some crude estimates).

27.2.2 Microlocal Analysis Unleashed

Sharp Estimates

Now we can unleash the full power of microlocal analysis but we need to extend it to our framework. It follows by induction from (27.2.28)–(27.2.29) and the arguments we used to derive these estimates that

$$\|\partial A\|_{\mathscr{C}^{n-\delta}} \le C_n \kappa h^{-1-n} \qquad \forall n\in \mathbb{Z}^+, \tag{27.2.31}$$

so A is "smooth" in $\varepsilon = h$ scale while for rough microlocal analysis as in Section 2.3 one needs at least $\varepsilon = Ch|\log h|$. We consider in this section arbitrary $d\ge 2$; see however Remark 27.2.9.

Proposition 27.2.10. *For a commutator of a pseudodifferential operator with a smooth symbol and* $\mathscr{C}^{\theta+1}$*-function* $A(x)$ *a usual commutator formula holds modulo* $O(h^{\theta+1}\|\!|\partial A|\!\|_\theta)$ *for any non-integer* $\theta>0$ *where*

$$\|\!|f|\!\|_\theta := \left\{\begin{aligned} &\sum_{\alpha:|\alpha|=\theta} \sup_x |\partial^\alpha f(x)| && \theta\in\mathbb{Z}^+,\\ &\sum_{\alpha:|\alpha|=\lfloor\theta\rfloor} \sup_{x\ne y} |x-y|^{\lfloor\theta\rfloor-\theta}\cdot |\partial^\alpha f(x)-\partial^\alpha f(y)| && \theta\notin\mathbb{Z}^+.\end{aligned}\right. \tag{27.2.32}$$

Proof. Easy proof is left to the reader. □

Proposition 27.2.11. *Assume that*

$$\|\partial V\|_{\mathscr{C}(B(0,2))} \le C_0 \tag{27.2.33}$$

and

$$\mu := \|\partial A\|_{\mathscr{C}(B(0,2))} \le C_0. \tag{27.2.34}$$

Let $U(x,y,t)$ *be the Schwartz kernel of* $e^{ih^{-1}tH_{A,V}}$*. Then for* $T\asymp 1$

(i) Estimate

$$\|F_{t\to h^{-1}\tau}\chi_T(t)(hD_x)^\alpha(hD_y)^\beta\psi_1(x)\psi_2(y)U\| \le Ch^s \tag{27.2.35}$$

holds for all $\alpha:|\alpha|\le 2$, $\beta:|\beta|\le 2$, s *and all* $\psi_1,\psi_2\in\mathscr{C}_0^\infty(B(0,1))$, *such that* $\mathsf{dist}(\mathsf{supp}(\psi_1),\mathsf{supp}(\psi_2))\ge C_0T$ *and* $\tau\le c_0$*; here* $\|.\|$ *means an operator norm from* $\mathscr{L}^2$ *to* $\mathscr{L}^2$*.*

(ii) Estimate

$$\|F_{t\to h^{-1}\tau}\chi_T(t)(hD_x)^\alpha(hD_y)^\beta\varphi_1(hD_x)\varphi_2(hD_y)U\| \le \\ Ch^s + Ch^\theta\bigl(\|\!|A|\!\|_{\theta+1}+\|\!|V|\!\|_{\theta+1}\bigr) \tag{27.2.36}$$

holds for all $\alpha:|\alpha|\le 2$, $\beta:|\beta|\le 2$, s *and all* $\varphi_1,\varphi_2\in\mathscr{C}_0^\infty$, *such that* $\mathsf{dist}(\mathsf{supp}(\varphi_1),\mathsf{supp}(\varphi_2))\ge C_0T$, *and* $\tau\le c_0$.

(iii) If also in $B(0,2)$

$$\epsilon_0\le|V|\le c \tag{27.2.37}$$

then for a small constant $T=\epsilon$ *estimate*

$$\|F_{t\to h^{-1}\tau}\chi_T(t)(hD_x)^\alpha(hD_y)^\beta U\| \le \\ Ch^s + Ch^\theta\bigl(\|\!|A|\!\|_{\theta+1}+\|\!|V|\!\|_{\theta+1}\bigr) \tag{27.2.38}$$

holds for all $\alpha:|\alpha|\le 2$, $\beta:|\beta|\le 2$, s *and all* $\psi_1,\psi_2\in\mathscr{C}_0^\infty(B(0,1))$, *such that* $\mathsf{diam}(\mathsf{supp}(\psi_1)\cup\mathsf{supp}(\psi_2))\le\epsilon_0T$ *and* $|\tau|\le\epsilon$.

Proof. Let $u=e^{ith^{-1}H}f$ with arbitrary $f\in\mathscr{L}^2$.

(i) Statement (i) is easily proven by the same arguments as in the proof of Theorem 2.1.2: we consider just usual function $\phi(x)$ and operators of multiplication like $\chi(\phi(x))$ so there are no "bad" commutators due to non-smoothness of A or V.

(ii) Statement (ii) is also proven by the same arguments; however in this case $\phi=\phi(x,\xi)$ so we need to involve "bad" commutators but their contributions are bounded by

$$C\|Q_1u\|\cdot\Bigl(h^{1+\theta}\bigl(\|\!|A|\!\|_{\theta+1}+\|\!|V|\!\|_{\theta+1}\bigr)\|u\|+h^{1+\delta}\|Q'u\|\Bigr)$$

in the right-hand expression while the left-hand expression is $\epsilon h\|Q_1 u\|^2$ where Q, Q_1, and Q' are operators with symbols $\chi(\phi(x,\xi))$, $\chi_1(\phi(x,\xi))$, and $\chi_1(\phi(x,\xi)-\eta)$ respectively, $\eta>0$ is an arbitrarily small constant (so the latter symbol has a bit larger support than the former one), $\delta>0$ is a small exponent, $\chi_1(t)=(-\chi'(t))^{\frac{1}{2}}$, and f.e. $\chi(t)=e^{-|t|^{-1}}$ for $t<0$, $\chi(t)=0$ for $t\geq 0$.

Therefore we conclude that

$$\|Qu\|\leq Ch^{\theta}\bigl(|||A|||_{\theta+1}+|||V|||_{\theta+1}\bigr)\|u\|+Ch^{\delta}\|Q'u\|$$

and similarly we can estimate $\|Q'u\|$ with $\|Q''u\|$ in the right-hand expression etc and thus we conclude that

$$\|Qu\|\leq Ch^{\theta}\bigl(|||A|||_{\theta+1}+|||V|||_{\theta+1}\bigr)\|u\|+Ch^{s}\|u\|$$

which is what we need.

(iii) Statement (iii) is easily proven by the same arguments as in the proof of Theorem 2.1.2: we consider just usual function $\phi(x)$ and operators of multiplication like $\chi(\phi(x))$ so there are no "bad" commutators due to non-smoothness of A or V. However we need to consider a contribution of u which is not confined to the small vicinity of (y,η) and we need Statement (ii) for this so the last term in the right-hand expression of (27.2.38) is inherited.

We leave easy details to the reader. □

Remark 27.2.12. In Proposition 27.2.11

(i) Statement (i) means the finite propagation speed with respect to x.

(ii) Statement (ii) means the finite propagation speed with respect to ξ and the last term in the right-hand expression of (27.2.36) is due to the non-smoothness of A and V.

(iii) Statement (iii) means that under assumption (27.2.37) there actually is a propagation with respect to x.

(iv) So far we have not assumed that V is very smooth function; we actually do not need it at all: it is sufficient to assume that ∂V is very smooth in the microscale $\varepsilon=h^{1-\delta}$; one can actually invoke more delicate arguments of the proof of Theorem 2.3.1 and deal with microscale $\varepsilon=Ch|\log h|$.

Therefore in the framework of Proposition 27.2.11(iii) estimate

$$|F_{t\to h^{-1}\tau}\chi_T(t)\bigl((hD_x)^\alpha(hD_y)^\beta U(x,y,t)\bigr)\bigr|_{x=y}| \le \\ Ch^{1-d+s}T^{-s}+CT^2h^{-d+\theta}\bigl(|\!|\!|A|\!|\!|_{\theta+1}+|\!|\!|V|\!|\!|_{\theta+1}\bigr) \tag{27.2.39}$$

holds for all $\alpha:|\alpha|\le 2$, $\beta:|\beta|\le 2$, s for $T=\epsilon$ and $|\tau|\le\epsilon$ where as usual $\chi\in\mathscr{C}_0^\infty([-1,-\frac{1}{2}]\cup[\frac{1}{2},1])$, $\chi_T(t)=\chi(t/T)$.

Let us consider $T\in(Ch,\epsilon)$; then we apply the standard rescaling $t\mapsto tT^{-1}$, $x\mapsto xT^{-1}$, $h\mapsto hT^{-1}$ and assumptions (27.2.33), (27.2.34) are replaced by weaker assumptions

$$T\|\partial V\|_{\mathscr{C}(B(x,1))}\le C_0 \tag{27.2.33$'$}$$

and

$$T\|\partial A\|_{\mathscr{C}(B(x,1))}\le C_0. \tag{27.2.34$'$}$$

Further, $|\!|\!|A|\!|\!|_{\theta+1}$ and $|\!|\!|V|\!|\!|_{\theta+1}$ acquire factor $T^{\theta+1}$.

Furthermore, since $U(x,y,t)$ is a density with respect to y we need to add factor T^{-d} to the right-hand expression and due to $F_{t\to h^{-1}\tau}$ we need to add another factor T and after these substitution and multiplications we arrive to

Proposition 27.2.13. *Let $h\le T\le\epsilon$ and assumptions* (27.2.33)$'$, (27.2.34)$'$ *and* (27.2.37) *be fulfilled. Then estimate* (27.2.39) *holds.*

Next we apply our standard arguments:

Proposition 27.2.14. *In the framework of Proposition 27.2.13 let $\bar\chi\in\mathscr{C}_0^\infty([-1,1])$. Then the following estimates hold:*

$$|F_{t\to h^{-1}\tau}\bigl[\bar\chi_T(t)\bigl((hD_x)^\alpha(hD_y)^\beta U(x,y,t)\bigr)\bigr]\bigr|_{x=y}| \le \\ Ch^{1-d}+CT^2h^{-d+\theta}\bigl(|\!|\!|A|\!|\!|_{\theta+1}+|\!|\!|V|\!|\!|_{\theta+1}\bigr) \tag{27.2.40}$$

and

$$|\bigl[\bigl((hD_x-A(x))\cdot\boldsymbol{\sigma}\bigr)^\alpha\bigl((hD_y-A(y))\cdot\boldsymbol{\sigma}\bigr)^\beta e(x,y,t)\bigr]\bigr|_{x=y}- \\ \mathsf{Weyl}_{\alpha,\beta}(x)|\le \\ Ch^{1-d}\bigl(1+\|\partial A\|_{\mathscr{C}(B(x,1))}+\|\partial V\|_{\mathscr{C}(B(x,1))}\bigr)+Ch^{-d+\frac{1}{2}(\theta+1)}\bigl(|\!|\!|A|\!|\!|_{\theta+1}+|\!|\!|V|\!|\!|_{\theta+1}\bigr)^{\frac{1}{2}} \tag{27.2.41}$$

where

$$\mathsf{Weyl}_{\alpha,\beta}(x) := \mathsf{const}\, h^{-d} \int_{\{H(x,\xi)\le\tau\}} \bigl((\xi - A(x))\cdot\boldsymbol{\sigma}\bigr)^{\alpha+\beta}\, d\xi \tag{27.2.42}$$

is the corresponding Weyl expression and

$$H(x,\xi) = \bigl((\xi - A(x))\cdot\boldsymbol{\sigma}\bigr)^2 - V(x); \tag{27.2.43}$$

in particular $\mathsf{Weyl}_{\alpha,\beta}(x) = 0$ *for* $|\alpha| + |\beta| = 1$.

Proof. Obviously, the summation of (27.2.39) over $C_0 h \le |t| \le T$ and a trivial estimate by Ch^{1-d} of the contribution of the interval $|t| \le C_0 h$ implies (27.2.40).

Then the standard Tauberian arguments imply that the left-hand expression of (27.2.41) does not exceed the right-hand expression of (27.2.40), divided by T, i.e.

$$CT^{-1}h^{1-d} + CTh^{-d+\theta}\bigl(\|\!|A|\!\|_{\theta+1} + \|\!|V|\!\|_{\theta+1}\bigr).$$

Optimizing with respect to $T \le \epsilon$, such that (27.2.33)$'$, (27.2.34)$'$ hold, we pick up $T = T^*$ with

$$T^* = \epsilon \min\Bigl(1,\ \bigl(\|\partial A\|_{\mathscr{C}(B(x,1))} + \|\partial V\|_{\mathscr{C}(B(x,1))}\bigr)^{-1},\ h^{-\frac{1}{2}(\theta-1)}\bigl(\|\!|A|\!\|_{\theta+1} + \|\!|V|\!\|_{\theta+1}\bigr)^{-\frac{1}{2}}\Bigr). \tag{27.2.44}$$

Meanwhile the Tauberian formula and (27.2.39) imply that the contribution of the interval $\{t : |t| \asymp T\}$ with $h \le T \le T^*$ to the Tauberian expression does not exceed the right-hand expression of (27.2.39) divided by T, i.e.

$$Ch^{1-d+s}T^{-s-1} + CTh^{-d+\theta}\|\partial A\|_{\mathscr{C}^\theta};$$

summation over $T_* := h^{1-\delta} \le T \le T^*$ results in the right-hand expression of (27.2.41).

So, we need to calculate only the contribution of $\{t : |t| \le T_*\}$ but one can see easily that modulo indicated error it coincides with $\mathsf{Weyl}_{\alpha,\beta}$. □

Remark 27.2.15. For $d \ge 3$ one can skip assumption (27.2.37).

Indeed, we can apply the standard rescaling technique: $x \mapsto x\ell^{-1}$, $h \mapsto \hbar = h\ell^{-\frac{3}{2}}$, $A \mapsto A\ell^{-\frac{1}{2}}$, $V \mapsto V\ell^{-1}$ with $\ell = \max(\epsilon|V|\nu^{-1},\ h^{\frac{2}{3}}\nu^{-\frac{1}{3}})$, $\nu = (1 + |\partial V|_{\mathscr{C}})$; see Section 5.2.

Application

Let us apply developed technique to estimate a minimizer.

Proposition 27.2.16. *Let $\kappa \le c$ and let A be a minimizer. Let*

$$\mu := \|\partial A\|_{\mathscr{C}} \le Ch^{-1+\delta}. \tag{27.2.45}$$

For $d=2$ let assumption (27.2.37) *be also fulfilled. Then for $\theta\in(1,2)$ estimate*

$$\|\partial A\|_{\mathscr{C}^{\theta-1}} + h^{\theta-1}\|\partial A\|_{\mathscr{C}^{\theta}} \le C\kappa\bigl(1+\|V\|_{\mathscr{C}^1} + h^{\frac{1}{2}(\theta-1)}\|V\|^{\frac{1}{2}}_{\mathscr{C}^{\theta+1}}\bigr) + C\|\partial A\|' \tag{27.2.46}$$

holds with

$$\|\partial A\|' := \sup_y \|\partial A\|_{\mathscr{L}^2(B(y,1))}. \tag{27.2.47}$$

Proof. Consider expression for ΔA. According to equation (27.2.14) and Proposition 27.2.14 $(|\Delta A| + |h\partial\Delta A|)$ does not exceed the right-hand expression of (27.2.41) multiplied by $C\kappa h^{d-1}$ i.e.

$$\|\Delta A\|_{\mathscr{C}} + \|h\partial\Delta A\|_{\mathscr{C}} \le C\kappa\Bigl(1 + |\partial A|_{\mathscr{C}} + |\partial V|_{\mathscr{C}} + h^{\frac{1}{2}(\theta-1)}\|\partial A\|^{\frac{1}{2}}_{\mathscr{C}^{\theta}} + h^{\frac{1}{2}(\theta-1)}\|\partial V\|^{\frac{1}{2}}_{\mathscr{C}^{\theta}}\Bigr), \tag{27.2.48}$$

where we replaced $|\!|\!| A|\!|\!|_{\theta+1}$ and $|\!|\!| V|\!|\!|_{\theta+1}$ by larger $\|\partial A\|_{\mathscr{C}^\theta}$ and $\|\partial V\|_{\mathscr{C}^\theta}$ respectively.

Then the regularity theory for elliptic equations implies that

(27.2.49) For any $\theta'\in(1,2)$ $h^{\theta'-1}\|\partial A\|_{\mathscr{C}^{\theta'}}$ does not exceed this expression (27.2.48) plus $C\|\partial A\|'$.

Observe that that $\|\partial A\|_{\mathscr{C}}$ does not exceed $(\epsilon\|\partial A\|_{\mathscr{C}^\theta} + C'_\epsilon\|\partial A\|')$ with arbitrarily small constant $\epsilon>0$ and therefore

$$h^{\theta-1}\|\partial A\|_{\mathscr{C}^\theta} + \epsilon^{-1}\|\partial A\|_{\mathscr{C}} \tag{27.2.50}$$

does not exceed expression (27.2.48) plus $C'_\epsilon\|\partial A\|'$ where we used (27.2.49) for $\theta'=\theta$.

Comparing (27.2.50) and (27.2.48) we conclude that for $\kappa\le c$ and sufficiently small constant $\epsilon>0$ we can eliminate in the derived inequality both contributions of ∂A to (27.2.48) thus we arrive to (27.2.46). □

Having this strong estimate to A allows us to prove

Theorem 27.2.17. *Let $\kappa \le c$, (27.2.45) be fulfilled, and let $d \ge 3$. Assume that*

$$\|V\|_{\mathscr{C}^{\theta+1}} \le c \tag{27.2.51}$$

with $\theta \in (1,2)$. Then

$$\mathsf{E}^* = \mathsf{Weyl}_1 + O(h^{2-d}) \tag{27.2.52}$$

and a minimizer A satisfies

$$\|\partial A\| \le C\kappa^{\frac{1}{2}} h^{\frac{1}{2}} \tag{27.2.53}$$

and

$$\|\partial A\|_{\mathscr{C}^{\theta-1}} + h^{\theta-1}\|\partial A\|_{\mathscr{C}^{\theta}} \le C\kappa^{\frac{1}{2}} h^{\frac{1}{2}} + C\kappa. \tag{27.2.54}$$

Proof. (a) In virtue of (27.2.40) the Tauberian error when calculating $\operatorname{Tr}(H^-_{A,V})$ does not exceed the right-hand expression of (27.2.40) multiplied by CT^{-2} i.e.

$$Ch^{1-d}T^{-2} + Ch^{-d+\theta}\bigl(|||A|||_{\theta+1} + |||V|||_{\theta+1}\bigr). \tag{27.2.55}$$

Assumption (27.2.51) allows us to simplify this expression and take $T \asymp (1+\mu)^{-1}$; applying estimate (27.2.46) we conclude that the Tauberian error does not exceed

$$C(1+\mu)^2 h^{2-d} + C(\kappa + \|\partial A\|')h^{2-d}. \tag{27.2.56}$$

We claim that

(27.2.57) Weyl error[5] when calculating $\operatorname{Tr}(H^-_{A,V})$ also does not exceed (27.2.56).

Then

$$\begin{gathered}\mathsf{E}(A) \ge \\ \mathsf{Weyl}_1 - C(1+\mu)^2 h^{2-d} - C(\kappa + \|\partial A\|')h^{2-d} + \kappa^{-1}h^{1-d}\|\partial A\|^2 \ge \\ \mathsf{Weyl}_1 - Ch^{2-d} + \frac{1}{2\kappa}h^{1-d}\|\partial A\|^2\end{gathered} \tag{27.2.58}$$

[5] I.e. error when we replace Tauberian expression by Weyl expression.

because $\mu \le C\|\partial A\|' + 1$ due to (27.2.46) and assumption (27.2.51). This implies an estimate of E^* from below and combining with the estimate $\mathsf{E}^* \le \mathsf{E}^*(0) = \mathsf{Weyl}_1 + Ch^{2-d}$ from above we arrive to (27.2.52) and (27.2.53) and then to (27.2.54) due to (27.2.46) and assumption (27.2.51).

(b) To prove (27.2.57) let us plug A_ε instead of A into $e_1(x,x,0)$. Then in virtue of the rough microlocal analysis the contribution to Weyl error of the interval $\{t : T_* \le |t| \le \epsilon\}$ with $T_* = h^{1-\delta}$ would be negligible and the contribution of the interval $\{t : |t| \le T_*\}$ would be $\mathsf{Weyl}_1 + O(h^{2-d})$.

(c) Now let us calculate an error which we made plugging A_ε instead of A into $e_1(x,x,0)$. Obviously it does not exceed $Ch^{-d}\|A - A_\varepsilon\|_{\mathscr{C}}$ and since $\|A - A_\varepsilon\|_{\mathscr{C}} \le C\varepsilon^{\theta+1}\|\partial A\|_{\mathscr{C}^\theta}$ this error does not exceed $Ch^{\theta+1-d-4\delta}\|\partial A\|_{\mathscr{C}^\theta}$, which is marginally worse than what we are looking for.

However it is good enough to recover a weaker version of (27.2.52) and (27.2.53) with an extra factor $h^{-\delta_1}$ in their right-hand expressions. Then (27.2.46) implies a bit weaker version of (27.2.54) and in particular that its left-hand expression does not exceed C.

Knowing this, let us consider the two term approximation. With the above knowledge one can prove easily that the error in two term approximation does not exceed $Ch^{3-d-\delta'}$ with $\delta' = 100\delta$.

Then the second term in the Tauberian expression is

$$\int \bigl((H_{A,V} - H_{A_\varepsilon,V})e^{\mathsf{T}}_{(\varepsilon)}(x,y,0)\bigr)\bigr|_{y=x}\,dx, \tag{27.2.59}$$

where subscript $_{(\varepsilon)}$ means that we plugged A_ε instead of A and superscript $^{\mathsf{T}}$ means that we consider Tauberian expression with $T = T^* = \epsilon$. But then the contribution of the interval $\{t : T_* \le |t| \le T^*\}$ is also negligible and modulo $Ch^{\theta+2-d-4\delta}\|\partial A\|_{\mathscr{C}^\theta}$ we get a Weyl expression. However

$$(H_{A,V} - H_{A_\varepsilon,V}) = -2(\xi - A_\varepsilon)\cdot(A - A_\varepsilon) + |A - A_\varepsilon|^2. \tag{27.2.60}$$

Observe that the first term in the right-hand expression kills the Weyl expression since an integrand is odd with respect to $(\xi - A_\varepsilon)$ while the second term as one can see easily makes it smaller than $Ch^{3-d-\delta'}$. Therefore (27.2.57) has been proven. □

Remark 27.2.18. (i) For $d = 2$ we cannot drop assumption (27.2.37) at this stage we did it for $d \ge 3$. However results of the next section allow us to cure this problem using the partition-and-rescaling technique.

(ii) Actually for $V\in \mathscr{C}^{2,1}$ we have an estimate

$$|\partial A(x)-\partial A(y)|\le C\kappa|x-y|(|\log|x-y||+1)+C\mu. \tag{27.2.61}$$

Combining with (27.2.53) we conclude that

$$\|\partial A\|_{\mathscr{C}}\le C\kappa^{(d+1)/(d+2)}|\log h|^{d/(d+2)}h^{1/(d+2)}. \tag{27.2.62}$$

(iii) If (27.2.51) holds for $(h\partial)^m V$ with $m\in \mathbb{Z}^+$ then (27.2.53) and (27.2.53) also hold for $(h\partial)^m A$ instead of A; further, if $(h\partial)^m V\in \mathscr{C}^{2,1}$ then (27.2.61) and (27.2.62) also hold for $(h\partial)^m A$ instead of A.

Classical Dynamics and Sharper Estimates

Now we want to improve the remainder estimate $O(h^{2-d})$ to $o(h^{2-d})$. Sure, we need to impose condition to the classical dynamical system and since $|\partial A|=O(h^\delta)$ with $\delta>0$ due to (27.2.62), it should be dynamical system associated with the Hamiltonian flow generated by $H_{0,V}$:

(27.2.63) The set of periodic points of the dynamical system associated with Hamiltonian flow generated by $H_{0,V}$ has measure 0 on the energy level 0.

Recall that on the energy level $\{(x,\xi): H_{0,V}(x,\xi)=\tau\}$ a natural density $d\mu_\tau = dxd\xi : dH|_{H=\tau}$ is defined.

The problem is we do not have a quantum propagation theory for $H_{A,V}$ as A is not a "rough" function (i.e. smooth in microscale ε). However it is a rather regular function, almost $\mathscr{C}^2$, and $(A-A_\varepsilon)$ is rather small: $|A-A_\varepsilon|\le \eta:=Ch^{2-3\delta}$ and $|\partial(A-A_\varepsilon)|\le Ch^{1-3\delta}$ and therefore we can apply a method of successive approximations with the unperturbed operator $H_{A_\varepsilon,V}$ as long as $\eta T/h\le h^\sigma$ i.e. as $T\le h^{1-4\delta}$. Here we, however, have no use for such large T and consider $T=O(h^{-\delta})$.

Consider

$$F_{t\to h^{-1}\tau}\chi_T(t)U(x,y,t), \tag{27.2.64}$$

and consider terms of successive approximations. Then if we forget about microhyperbolicity arguments the first term will be $O(h^{-d}T)$, the second term $O(h^{-1-d}\eta T^2)=O(h^{1-d-\delta'})$ and the error term $O(h^{-2-d}\eta^2T^3)=O(h^{2-d-\delta''})$.

Therefore since our goal is $O(h^{1-d})$ we need to consider the first two terms only. The first term is the same expression (27.2.64) with U replaced by $U_{(\varepsilon)}$.

Consider the second term, it corresponds to $U'_{(\varepsilon)}(x,y,t)$ which is the Schwartz kernel of operator

$$\mathsf{U}'_{(\varepsilon)} := ih^{-1}\int_0^t e^{i(t-t')h^{-1}H_{A_\varepsilon,V}}\bigl(H_{A,V}-H_{A_\varepsilon,V}\bigr)e^{it'h^{-1}H_{A_\varepsilon,V}}\,dt' \tag{27.2.65}$$

and then

$$\operatorname{Tr}\bigl(\mathsf{U}'_{(\varepsilon)}\psi\bigr) = ih^{-1}\operatorname{Tr}\Bigl(\bigl(H_{A,V}-H_{A_\varepsilon,V}\bigr)e^{ih^{-1}tH_{A_\varepsilon,V}}\psi^1(t)\Bigr) \tag{27.2.66}$$

where

$$\psi^1(t) := \int_0^t e^{ih^{-1}t'H_{A_\varepsilon,V}}\psi e^{-ih^{-1}t'H_{A_\varepsilon,V}}\,dt'$$

is h-pseudodifferential operator with a rough symbol and $\psi^1(t)\sim t$.

Really, one can prove easily studying first the Hamiltonian flow equation and then the transport equations that $\psi_t := e^{ih^{-1}tH_{A_\varepsilon,V}}\psi e^{-ih^{-1}tH_{A_\varepsilon,V}}$ is a h-pseudodifferential operator with a rough symbol and its corresponding norm is bounded.

Note that

$$ih^{-1}F_{t\to h^{-1}\tau}e^{ih^{-1}tH_{A_\varepsilon,V}}\psi^1(t) = (2\pi)\int\bigl(F_{t\to h^{-1}\tau'}e^{ih^{-1}tH_{A_\varepsilon,V}}\bigr)\hat{f}(h^{-1}(\tau-\tau'))\,d\tau'$$

with $\hat{f}=F_{t\to\tau}f_t$, $f_t=\chi_T(t)\psi^1(t)$ and therefore (27.2.65)–(27.2.66) imply that

$$|F_{t\to h^{-1}\tau}\chi_T(t)\operatorname{Tr}\mathsf{U}'_{(\varepsilon)}\psi| \le C\eta T^2h^{-d} \tag{27.2.67}$$

where in comparison with the trivial estimate we gained the factor h.

We can plug here $T'\in(T_*,T)$ instead of T and, taking summation by T' from $T_*=\epsilon$ to T, we conclude that estimate (27.2.67) also holds for $\chi_T(t)$ replaced by $\bigl(\bar\chi_T(t)-\bar\chi_{T_*}(t)\bigr)$ (provided $\bar\chi=1$ on $(-\frac{1}{2},\frac{1}{2})$) and since $\eta T^2\le h^{1+\delta}$ for $T\le h^{-\delta}$ we see that the right-hand expression (27.2.67) does not exceed $Ch^{1-d+\delta}$.

On the other hand, our traditional methods imply that

$$|F_{t\to h^{-1}\tau}\chi_T(t)\operatorname{Tr}\bigl(e^{ith^{-1}H_{A_\varepsilon,V}}\psi\bigr)| \le Ch^{1-d}T\upmu(\Pi_{T,\zeta})+C_{T,\zeta}h^{1-d+\delta} \tag{27.2.68}$$

where Π_T is the set of points on energy level 0, periodic with periods not exceeding T, $\Pi_{T,\zeta}$ is its ζ-vicinity, $\zeta>0$ is arbitrarily small; recall that for $d=2$ we assume that condition (27.2.37) is fulfilled.

Here again we can plug any $T'\in (T_*,T)$ instead of T and after summation with respect to T' we conclude that (27.2.68) also holds with $\chi_T(t)$ replaced by $\bigl(\bar\chi_T(t)-\bar\chi_{T_*}(t)\bigr)$.

Combining with estimate for $\bigl(e^{ith^{-1}H_{A_\varepsilon,V}}-e^{ith^{-1}H_{A_\varepsilon,V}}\bigr)$ we conclude that

$$|F_{t\to h^{-1}\tau}\bigl(\bar\chi_T(t)-\bar\chi_{T_*}(t)\bigr)\operatorname{Tr}\bigl(e^{it'h^{-1}H_{A,V}}\psi\bigr)|\le\\ Ch^{1-d}T\upmu(\Pi_{T,\zeta})+C_{T,\zeta}h^{1-d+\delta}$$

and since

$$|F_{t\to h^{-1}\tau}\bar\chi_{T_*}(t)\operatorname{Tr}\bigl(e^{it'h^{-1}H_{A,V}}\psi\bigr)|\le Ch^{1-d}$$

we conclude that

$$|F_{t\to h^{-1}\tau}\bar\chi_T(t)\operatorname{Tr}\bigl(e^{it'h^{-1}H_{A,V}}\psi\bigr)|\le\\ Ch^{1-d}+Ch^{1-d}T\upmu(\Pi_{T,\zeta})+C_{T,\zeta}h^{1-d+\delta}. \tag{27.2.69}$$

Then the Tauberian error does not exceed the right-hand expression of (27.2.69) multiplied by ChT^{-2} and it is less than $CT^{-1}h^{2-d}$.

Consider now the Tauberian expression and again apply the two-term approximation for $e^{ih^{-1}tH_{A,V}}$ considering $e^{ih^{-1}tH_{A_\varepsilon,V}}$ as an unperturbed operator; then the error will be less than $Ch^{2-d+\delta}$.

Consider the second term after taking trace; it is $O(h^{2-d-4\delta})$, so it is just slightly too large. Further, if $\psi=I$ one can calculate it easily and observe that it is $O(h^{2-d+\delta})$ provided $V\in\mathscr{C}^{2,1}$.

Finally, the first term is what we get for $e^{ih^{-1}tH_{A_\varepsilon,V}}$ and in virtue of rough microlocal analysis the contribution of the interval $\{t\colon T_*\le|t|\le T\}$ does not exceed $Ch^{2-d}\upmu(\Pi_{T,\zeta})+C_{T,\zeta}h^{2-d+\delta}$ and the contribution of the interval $\{t\colon |t|\le T_*\}$ is $\mathsf{Weyl}_1+O(h^{2-d+\delta})$.

Then we arrive to

Theorem 27.2.19. *Let $\kappa\le c$,* (27.2.45) *and* (27.2.51) *be fulfilled. Furthermore, let condition* (27.2.63) *be fulfilled*[6]*. Then*

$$\mathsf{E}^*=\mathsf{Weyl}_1^*+o(h^{2-d}) \tag{27.2.70}$$

where

$$\mathsf{Weyl}_1^*=\mathsf{Weyl}_1+\varkappa h^{2-d}\int V_+^{\frac{d}{2}}\Delta V\,dx \tag{27.2.71}$$

calculated in the standard way for $H_{0,V}$ and a minimizer A satisfies similarly improved versions of (27.2.53) *and* (27.2.54).

[6] I.e. $\upmu_0(\Pi_\infty)=0$.

Remark 27.2.20. (i) Recall that for $d=2$ so far we assume (27.2.37). However we need it only to estimate ∂A. Indeed, even in the case of very degenerate potential V the "magnetic" correction will be small since $|\partial A|$ is small.

(ii) Under stronger assumptions to the Hamiltonian flow one can recover better estimates like $O(h^{2-d}|\log h|^{-2})$ or even $O(h^{2+\delta-d})$ (like in Subsubsection 4.5.4.3 *Sharper Remainder Estimates*).

(iii) We leave to the reader to calculate the numerical constants $\varkappa_*$ here and in (27.2.76) below, $\varkappa=\varkappa_1-\frac{2}{d}\varkappa_2$.

(iv) However, even if $\psi\ne I$ we can observe that it is sufficient to consider only principal terms and then the second term in approximations is also $O(h^{2-d+\delta})$ provided $V\in\mathscr{C}^{2,1}$ as long as principal symbol of $\psi(x)$ is even with respect to ξ, in particular, if $\psi=\psi(x)$.

27.2.3 Local Theory

Localization and Estimate from above

The results of the previous Subsection 27.2.2 have two critical shortcomings: first, they impose the excessive initial requirement (27.2.21) to κ as we need to start from $M\le ch^{-3}$; second, they are not local. However, curing the second shortcoming, we make the way to addressing the first one as well, using the partition and rescaling technique.

We can localize $\mathsf{Tr}^-(H)=\mathsf{Tr}(H^-)$, which is the first term in $\mathsf{E}(A)$, either in our traditional way as $\mathsf{Tr}(H^-\psi^2)$ or in the way favored by some mathematical physicists[7]: namely, we take $\mathsf{Tr}^-(\psi H\psi)$ where in both cases $\psi\in\mathscr{C}_0^\infty(B(0,\frac{1}{2}))$, $0\le\psi\le 1$ and some other conditions will be imposed to it later. Observe that

$$\mathsf{Tr}^-(\psi H\psi)\ge\mathsf{Tr}(\psi H^-\psi)=\int e_1(x,x,0)\psi^2(x)\,dx. \tag{27.2.72}$$

Really, let us decompose operator $H=H\theta(-H)+H(1-\theta(-H))$, where $\theta(\tau-H)$ is a spectral projector of H, and therefore in the operator sense $H\ge H^-:=H\theta(-H)$ and $\psi H\psi\ge\psi H^-\psi$, and therefore all negative eigenvalues

[7] See f. e. L. Erdös, S. Fournais. and J. P. Solovej [4].

of $\psi H\psi$ are greater than or equal to eigenvalues of the negative operator $\psi H^-\psi$, and then

$$\mathsf{Tr}^-(\psi H\psi) \ge \mathsf{Tr}(\psi H^-\psi) = \mathsf{Tr}\Bigl(\int_{-\infty}^{0} \tau d_\tau \theta(\tau - H)\psi^2\Bigr), \tag{27.2.73}$$

which is exactly the right-hand expression of (27.2.72).

Remark 27.2.21. Each approach has its own advantages.

(i) In particular, no need to localize A (see (ii)) and the fact that Proposition 27.2.5 obviously remains true are advantages of $\mathsf{Tr}^-(\psi H\psi)$-localization.

(ii) Further, sinces $\mathsf{Tr}^-(\psi H\psi)$ does not depend on A outside of $B(0,\frac{3}{4})$ we may assume that $A=0$ outside of $B(0,1)$. Really, we can always subtract a constant from A without affecting traces and also cut-off A outside of $B(0,1)$ in a way such that $A'=A$ in $B(0,\frac{3}{4})$ and $\|\partial A'\| \le c\|\partial A\|_{B(0,1)}$; the price is to multiply κ by c^{-1}–as long as principal parts of asymptotics coincide.

(iii) On the other hand, additivity rather than sub-additivity of (27.2.88) and the trivial estimate from the above are advantages of $\mathsf{Tr}(\psi H^-\psi)$-localization; therefore it is more advantageous.

(iv) In the next Chapter 28 (in Section 28.2) we will use more $\mathsf{Tr}^-(\psi H\psi)$-localization for preliminary estimates from below and simplify many arguments of this Section. We apply these modifications and simplifications to this Section in the final version of the Book.

We will use both methods and here we provide an upper estimate for the larger expression $\mathsf{Tr}^-(\psi H\psi)$ and a lower estimate for the lesser expression $\mathsf{Tr}(\psi H^-\psi)$. Let us estimate from the above:

Proposition 27.2.22. *Assume that $V\in\mathscr{C}^{2,1}$, $d\ge 2$. Let $\ell(x)$ be a scaling function*[8] *and ψ be a function such that $|\partial^\alpha\psi|\le c\psi\ell^{-\sigma|\alpha|}$ for all $\alpha:|\alpha|\le 2$ and $|\psi|\le c\ell^{\sigma(1+\delta)}$ with $\sigma>1$ and $\delta>0$*[9]*.*

Then, if $A=0$,

$$\mathsf{Tr}^-(\psi H\psi) = \int \mathsf{Weyl}_1(x)\psi^2(x)\,dx + O(h^{2-d}) \tag{27.2.74}$$

[8] I.e. $\ell\ge 0$ and $|\partial\ell|\le\frac{1}{2}$.

[9] Such compactly supported functions obviously exist.

and under assumption (27.2.63)

$$\mathsf{Tr}^-(\psi H\psi) = \int \mathsf{Weyl}_1^*(x)\psi^2(x)\,dx + o(h^{2-d}) \tag{27.2.75}$$

with

$$\mathsf{Weyl}_1^*(x) = \mathsf{Weyl}_1(x) + \varkappa_1 h^{-1} V_+^{\frac{d}{2}}\Delta V + \varkappa_2 h^{-1} V_+^{\frac{d}{2}-1}|\nabla V|^2 \tag{27.2.76}$$

calculated in the standard way for $H_{0,V}$.

Proof. Let us consider $\tilde{H} = \psi H\psi$ as a Hamiltonian and let $\tilde{e}(x,y,\tau)$ be the Schwartz kernel of its spectral projector. Then

$$\mathsf{Tr}^-(\psi H\psi) = \int \tilde{e}_1(x,x,0)\,dx = \sum_j \int \tilde{e}_1(x,x,0)\psi_j^2\,dx, \tag{27.2.77}$$

where ψ_j^2 form a partition of unity in $\mathbb{R}^d$ and we need to calculate the right hand expression. The problem is that $\tilde{H}$ is not a usual Schrödinger operator because of the degenerating factor ψ on each side.

Consider first an $\epsilon\ell$-admissible partition of unity in $B(0,1)$. Let us consider γ-scale in such element where $\gamma = \epsilon\ell^\sigma$ and we will use 1-scale in ξ. Then after rescaling $x \mapsto x\gamma^{-1}$ the semiclassical parameter rescales $h \mapsto h_{\mathsf{new}} = h\gamma^{-1}$ and the contribution of each γ-subelement to a semiclassical remainder does not exceed $C\psi^2(h/\gamma)^{2-d}$ with $\psi \le \gamma^{1+\delta}$, having the same magnitude over element as long as $\gamma \ge 2h$. Then the contribution of ℓ-element to a semiclassical error does not exceed $C\psi^2(h/\gamma)^{2-d}\times \ell^d\gamma^{2-d} \asymp Ch^{2-d}\psi^2\gamma^{-2}\ell^d \le Ch^{2-d}\ell^{d+2\delta}$.

Note that expression (27.2.77) only increases if we sum only with respect to elements where $\ell^\sigma \ge h$. Therefore we arrive to estimate

$$\mathsf{Tr}^-(\psi H\psi) \le \int \mathsf{Weyl}_1(x)\psi^2(x)\,dx + Ch^{2-d},$$

where integration is taken over a domain $\{x\colon \ell(x) \ge h^{1/\sigma}\}$. Note that we can extend this integral to $\mathbb{R}^d$: indeed, it will add negative term with absolute value not exceeding $Ch^{-d}\times h^{2+\delta}$ as $\psi \le h^{1+\delta}$ there and it is absorbed by the remainder estimate. □

Corollary 27.2.23. *In the framework of Proposition 27.2.22*

$$\mathsf{E}^*_\psi := \inf_A \mathsf{E}_\psi(A) \le \int \mathsf{Weyl}_1(x)\psi^2(x)\,dx + Ch^{2-d} \tag{27.2.78}$$

and under assumption (27.2.63)

$$\mathsf{E}^*_\psi \le \int \mathsf{Weyl}_1(x)\psi^2(x)\,dx + Ch^{2-d} \tag{27.2.79}$$

with

$$\mathsf{E}_\psi(A) := \mathsf{Tr}^-(\psi H\psi) + \frac{1}{\kappa h^2}\int |\partial A|^2\,dx. \tag{27.2.80}$$

Proof. Indeed, we just pick $A = 0$. ☐

Estimate from below

Now let us estimate *redefined* $\mathsf{E}_\psi(A)$,

$$\mathsf{E}_\psi(A) := \int e_1(x,x,0)\psi^2(x)\,dx + \frac{1}{\kappa h^{d-1}}\int |\partial A|^2\,dx, \tag{27.2.81}$$

from below. However we need an equation for an optimizer and it would be easier for us to deal with even lesser expression involving τ-regularization. Let us rewrite the first term in the right-hand expression in the form

$$\int_{-\infty}^0 \bar\varphi(\tau/L)\tau\, d_\tau e(x,x,\tau) + \int_{-\infty}^0 (1-\bar\varphi(\tau/L))\tau\, d_\tau e(x,x,\tau) \ge \\ \int_{-\infty}^L \Bigl(\bar\varphi(\tau/L)(\tau - L)\, d_\tau e(x,x,\tau) + (1-\bar\varphi(\tau/L))\tau\, d_\tau e(x,x,\tau)\Bigr),$$

where $\bar\varphi \in \mathscr{C}_0^\infty([-1,1])$ equals 1 in $[-\frac{1}{2},\frac{1}{2}]$ and let us estimate from below

$$\mathsf{E}'_\psi(A) := \int \Bigl(\int_{-\infty}^L \bar\varphi(\tau/L)(\tau-L)d_\tau e(x,x,\tau)(x) + \\ (1-\bar\varphi(\tau/L))(\tau-L)\,d_\tau e(x,x,\tau)\Bigr)\psi^2(x)\,dx + \frac{1}{kh^{1-d}}\int |\partial A|^2\,dx. \tag{27.2.82}$$

Let us generalize Proposition 27.2.4:

Proposition 27.2.24. *Let A be a minimizer of $\mathsf{E}'_\psi(A)$. Then*

$$\frac{2}{\kappa h^{1-d}}\Delta A_j(x) = \Phi_j := \\ \operatorname{Re}\operatorname{tr}\Bigl[\sigma_j\Bigl((hD-A)_x\cdot\boldsymbol{\sigma}\mathcal{K}(x,y,\tau) + \mathcal{K}(x,y,\tau)\,{}^t(hD-A)_y\cdot\boldsymbol{\sigma}\Bigr)\Bigr]\Bigr|_{y=x} \tag{27.2.83}$$

with

$$\mathcal{K}=\int_{-\infty}^{L}\mathsf{SK}\Big[\bar{\varphi}(\tau/L)(\tau-L)\operatorname{Res}_{\mathbb{R}}(\tau-H)^{-1}\psi^2(\tau-H)^{-1}+ \\ (1-\bar{\varphi}(\tau/L))\tau(\tau-L)\operatorname{Res}_{\mathbb{R}}(\tau-H)^{-1}\psi^2(\tau-H)^{-1}\Big](x,y)\,d\tau,$$

where we use a temporary notation $\mathsf{SK}[B](x,y)$ *for the Schwartz kernel of operator* B*.*

Proof. Follows immediately from the proof of Proposition 27.2.4. □

Proposition 27.2.25. *Let* $d=3$ *and assumptions* (27.2.20) *and* (27.2.21) *be fulfilled. Then for* $\tau\le c$

(i) Operator norm in $\mathscr{L}^2$ *of* $(hD)^k(\tau-H)^{-1}$ *does not exceed* $C|\operatorname{Im}\tau|^{-1}$ *for* $k=0,1,2;$*.*

(ii) Operator norm in $\mathscr{L}^2$ *of* $(hD)^2\big((hD-A)\cdot\boldsymbol{\sigma}\big)(\tau-H)^{-1}$ *does not exceed* $C|\operatorname{Im}\tau|^{-1}$ *for* $k=0,1,2$*.*

Proof. Proof follows the same scheme as the proof of Proposition 27.2.6. □

Proposition 27.2.26. *Let* $d=3$ *and assumptions* (27.2.20) *and* (27.2.21) *be fulfilled. Then* $|\Phi(x)|\le Ch^{-3}$*.*

Proof. Let us estimate

$$|\int\tau\varphi(\tau/L)\operatorname{Res}_{\mathbb{R}}\mathsf{SK}\Big[Q(\tau-H)^{-1}\psi^2(\tau-H)^{-1}\Big](x,y)\,d\tau|, \tag{27.2.84}$$

where $L\le c$ and $\varphi\in\mathscr{C}_0^\infty([-1,1])$ and also a similar expression with a factor $(\tau-L)$ instead of τ; here either $Q=I$, or $Q=(hD_k-A_k)_x$ or $Q=(hD_k-A_k)_y$.

Proposition 27.2.25 implies that the Schwartz kernel of the integrand does not exceed $Ch^{-3}|\operatorname{Im}\tau|^{-2}$ and therefore expression (27.2.84) does not exceed $CL^2\times h^{-3}L^{-2}=Ch^{-3}$.

Then what comes out in Φ from the term with the factor $\bar{\phi}(\tau/h)$ does not exceed Ch^{-3}.

Then, representing $\big(1-\bar{\phi}(\tau/h)\big)$ as a sum of $\varphi(\tau/L)$ with $L=2^nh$ with $n=0,\dots,\lfloor|\log h|\rfloor+c$, we estimate the output of each term by Ch^{-3} and thus the whole sum by $Ch^{-3}|\log h|$.

To get rid of the logarithmic factor we use equality

$$(\tau - H)^{-1}\psi(\tau - H)^{-1} = - \partial(\tau - H)^{-1}\psi + (\tau - H)^{-2}[h, \psi](\tau - H)^{-1}; \tag{27.2.85}$$

if we plug only the second part, we recover a factor h/L, where h comes from the commutator and $1/L$ from the increased singularity; an extra operator factor in the commutator is not essential. Then summation over partition results in Ch^{-3}.

Plugging only the first part we do not use the above decomposition but the equality $\mathsf{Res}_{\mathbb{R}}(\tau - H)^{-1}\, d\tau = d_\tau \theta(\tau - H)$. □

Corollary 27.2.27. *Let* $d = 3$, *assumptions* (27.2.20) *and* (27.2.21) *be fulfilled and* A *be a minimizer. Then* (27.2.28) *and* (27.2.29) *hold.*

Proof. Proof follows the proof of Corollary 27.2.8. □

Now we can recover both Proposition 27.2.16 and our both main Theorems 27.2.17 and 27.2.19:

Theorem 27.2.28. *Let* $d = 3$ *and assumptions* (27.2.20) *and* $\kappa \le c$ *be fulfilled. Then*

(i) The following estimate holds:

$$\mathsf{E}^*_\psi - \int \mathsf{Weyl}_1(x)\psi^2(x)\, dx = O(h^{2-d}) \tag{27.2.86}$$

and and a minimizer A *satisfies* (27.2.53) *and* (27.2.54).

(ii) Furthermore, let assumption (27.2.63) *be fulfilled (i.e.* $\mu_0(\Pi_\infty) = 0$*). Then*

$$\mathsf{E}^*_\psi - \int \mathsf{Weyl}^*_1(x)\psi^2(x)\, dx = o(h^{2-d}) \tag{27.2.87}$$

and a minimizer A *satisfies similarly improved versions of* (27.2.53) *and* (27.2.54).

27.2.4 Rescaling

Now we apply the rescaling. We consider only $d = 3$ here.

Case $\kappa \le 1$

We already have an upper estimate: see Corollary 27.2.23. Let us prove a lower estimate[10]. Consider an error

$$\Bigl(\int \mathsf{Weyl}_1(x)\psi^2\,dx - \mathsf{E}_\psi(A)\Bigr)_+. \tag{27.2.88}$$

Obviously, Tr^- is sub-additive

$$\mathsf{Tr}^-(\sum_j \psi_j H\psi_j) \ge \sum_j \mathsf{Tr}^-(\psi_j H\psi_j), \tag{27.2.89}$$

and therefore so is $\mathsf{E}_\psi(A)$ under assumption that $\psi_j \in \mathscr{C}_0^2(B(x_j, \frac{1}{2}\ell_j))$, where multiplicity of covering by $B(x_j,\ell_j))$ does not exceed C_0 and we are allowed to replace κ by $C_1\kappa$ in the right-hand expression[11].

Then we need to consider each partition element and use a lower estimate for it. While considering partition we use so called *ISM identity*: if

$$\sum_j \psi_j^2 = 1, \tag{27.2.90}$$

we have

$$H = \sum_j \bigl(\psi_j H\psi_j + \frac{1}{2}[[H,\psi_j],\psi_j]\bigr) = \sum_j \psi_j\bigl(H + \frac{1}{2}\sum_k [[H,\psi_k],\psi_k]\bigr)\psi_j, \tag{27.2.91}$$

where the second equality is due to the fact that $[[H,\psi_j],\psi_j]$ is an ordinary function.

In virtue of Proposition 27.2.5, from the very beginning we need to consider

$$M = \kappa^\beta h^{-1-\alpha} \tag{27.2.92}$$

with $\alpha = 2$, $\beta = 0$ and $\kappa \le c$. But we need to satisfy precondition (27.2.21) which is then

[10] But only for $\mathsf{E}_\psi(A)$ defined by (27.2.80).

[11] Really, $\|\partial A\|^2 \ge c\sum_j \|\partial A_j\|^2$ with $A_j(x) = (A(x) - A_j(x_j))\psi'_j$ with $\psi'_j \in \mathscr{C}_0^2(B(x_j, \frac{7}{8}\ell_j))$ equal 1 in $B(x_j, \frac{3}{4}\ell_j))$.

$$\kappa^{\beta+1} h^{-\alpha} \le c. \tag{27.2.93}$$

Therefore, if condition (27.2.93) is fulfilled with $\alpha = 0$, we conclude that the final error is indeed $O(h^{-1})$ or even $o(h^{-1})$ (under assumption (27.2.63)) without any precondition.

Let precondition (27.2.93) fail. Let us use γ-admissible partition of unity ψ_j^2 with ψ_j satisfying after rescaling assumptions of Proposition 27.2.22.

Note that rescaling $x \mapsto x\gamma^{-1}$ results in $h \mapsto h_{\mathsf{new}} = h\gamma^{-1}$ and after rescaling in the new coordinates $\|\partial A\|^2$ acquires factor γ^{d-2} and thus factor $\kappa^{-1}h^{-2}$ becomes $\kappa^{-1}h^{-2}\gamma^{d-2} = \kappa_{\mathsf{new}}^{-1}h_{\mathsf{new}}^{-2}$ with $\kappa \mapsto \kappa_{\mathsf{new}} = \kappa\gamma$.

Then *after rescaling* precondition (27.2.93) is satisfied provided *before rescaling* $\kappa^{\beta+1}h^{-\alpha}\gamma^{\alpha+\beta+1} \le c$. Thus, let us pick up the largest γ satisfying this: $\gamma = \kappa^{-(\beta+1)/(\alpha+\beta+1)}h^{\alpha/(\alpha+\beta+1)}$. Obviously, if before rescaling condition (27.2.93) fails, then $h \ll \gamma \le 1$.

But then expression (27.2.88) with ψ replaced by ψ_j does not exceed $Ch_{\mathsf{new}}^{-1} = C(h\gamma^{-1})^{-1}$ and the total expression (27.2.88) does not exceed $C(h\gamma^{-1})^{-1}\gamma^{-3} = Ch^{-1}\gamma^{-2} = C\kappa^{\beta'}h^{-1-\alpha'}$ with

$$\beta' = 2(\beta+1)/(\alpha+\beta+1), \qquad \alpha' = 2\alpha/(\alpha+\beta+1).$$

Therefore, actually we can pick up M with α, β replaced by α', β' and we have a precondition (27.2.93) with these new α', β' and we do not need an old precondition. Repeating the rescaling procedure again, we derive a proper estimate with again weaker precondition etc.

One can see easily that $\alpha' + \beta' + 1 = 3$ and therefore on each step $\alpha + \beta + 1 = 3$ and we have a recurrent relation for α': $\alpha' = \frac{2}{3}\alpha$; and therefore we have sequence for α which decays and becomes arbitrarily small. Therefore precondition (27.2.93) has been reduced to a much weaker assumption $\kappa \le h^{\delta}$ and under it estimate $M = O(h^{-1})$ has been established. Furthermore, after this under assumption (27.2.63) we can prove even sharper asymptotics.

To weaken assumption $\kappa \le h^{\delta}$ to $\kappa \le c$ we can use rescaling $x \mapsto x\gamma^{-1}$ with $\gamma = h^{\delta}$. We arrive to the error estimate $O(h^{-1-\delta})$ and therefore optimizer satisfies $\|\nabla \times A\| \le h^{\frac{1}{2}-\delta}$ (where δ is increased if necessary but remains arbitrarily small). Repeating the arguments of the proof of Proposition 27.2.6, instead of $\|\Delta A\|_{\mathscr{L}^\infty} = O(1)$ we arrive to $\|\Delta A\|_{\mathscr{L}^\infty} = O(h^{-\delta})$ and to $\|\partial^2 A\|_{\mathscr{L}^\infty} = O(h^{-\delta})$; then $\|\partial A\|_{\mathscr{L}^\infty} = O(h^{\frac{1}{2}-\delta})$; it is more than sufficient to unleash the microlocal analysis technique without any need to appeal to Proposition 27.2.6 which is the only place where we needed assumption (27.2.21).

Thus we arrive to

Theorem 27.2.29. *Let $d=3$, $V\in\mathscr{C}^{2,1}$, $\kappa\le c$ and let ψ satisfy assumption of Proposition 27.2.22. Then*

(i) Asymptotics (27.2.86) *holds.*

(ii) Further, if assumption (27.2.63) *is fulfilled then asymptotics* (27.2.86) *holds.*

(iii) If (27.2.86) *or* (27.2.87) *holds for $E_\psi(A)$ (we need only an estimate from below) then $\|\partial A\| = O((\kappa h)^{\frac{1}{2}})$ or $\|\partial A\| = o((\kappa h)^{\frac{1}{2}})$ respectively.*

Case $1\le\kappa\le h^{-1}$

In this framework we can consider even the case $1\le\kappa\le h^{-1}$. The simple rescaling-and-partition arguments with $\gamma=\kappa^{-1}$ lead to the following

(27.2.94) If $1\le\kappa\le h^{-1}$, then the remainder estimate $O(\kappa^2h^{-1})$ holds and for a minimizer A satisfies $\|\partial A\|^2\le C\kappa^3 h$.

However we would like to improve it and, in particular, to prove that if κ is moderately large then the remainder estimate is still $O(h^{-1})$ and even $o(h^{-1})$ under non-periodicity assumption.

Theorem 27.2.30. *Let $d=3$, $V\in\mathscr{C}^{2,1}$, and let ψ satisfy assumptions of Proposition 27.2.22. Then*

(i) For

$$\kappa\le\kappa_h^* := \epsilon h^{-\frac{1}{4}}|\log h|^{-\frac{3}{4}} \tag{27.2.95}$$

asymptotics (27.2.86) *holds.*

(ii) Furthermore, for $\kappa=o(\kappa_h^*)$ and assumption (27.2.63) *is fulfilled then asymptotics* (27.2.87) *holds.*

(iii) If $\kappa_h^*\le\kappa\le ch^{-1}$ the following estimate holds:

$$|\mathsf{E}^*_\psi - \int \mathsf{Weyl}_1(x)\psi^2(x)\,dx| \le Ch^{-3}(\kappa h)^{\frac{8}{3}}|\log \kappa h|^2. \tag{27.2.96}$$

Proof. (i) From (27.2.46) we conclude for $\kappa \ge c$ that

$$h^{1-\theta}|\partial A|_{\mathscr{C}^\theta} \le C\kappa(\kappa+\bar{\mu}).$$

Then, using arguments of Subsection 27.2.2, one can prove easily that for $\kappa \le h^{\sigma-\frac{1}{2}}$

$$|F_{t\to h^{-1}\tau}\bar{\chi}_T(t)(hD_x)^\alpha(hD_x)^\beta\bigl(U(x,y,t)-U_{(\varepsilon)}(x,y,t)-U'_{(\varepsilon)}(x,y,t)\bigr)| \le Ch^{1-d},$$

where we use the same 2-term approximation, $T=\epsilon\bar{\mu}^{-1}$. Let us take then $x=y$, multiply by $\varepsilon^{-d}\psi(\varepsilon^{-1}(y-z))$ and integrate over y. Using the rough microlocal analysis technique, one can prove easily that from both $U_{(\varepsilon)}(x,y,t)$ and $U'_{(\varepsilon)}(x,y,t)$ we get $O(h^{-2})$ and in the end of the day we arrive to the estimate $|\Delta A_\varepsilon| \le C\kappa\bar{\mu}$, which implies

$$|\partial^2 A_\varepsilon| \le C\kappa\bar{\mu}|\log h| + C\mu, \tag{27.2.97}$$

where obviously one can skip the last term. Here we used the regularity property of the Laplace equation. For our purpose it is much better than the estimate $|\partial^2 A_\varepsilon| \le C\kappa^2|\log h| + C\mu$, which one could derive easily.

Again, using arguments of Subsection 27.2.2, one can prove easily that

$$|\operatorname{Tr}(\psi H^-_{A,V}\psi) - \operatorname{Tr}(\psi H^-_{A_\varepsilon,V}\psi)| \le C\bar{\mu}^2h^{2-d} \tag{27.2.98}$$

and therefore

$$|\operatorname{Tr}(\psi H^-_{A,V}\psi) - \int \mathsf{Weyl}_1(x)\psi^2(x)\,dx| \le C\bar{\mu}^2h^{2-d} \tag{27.2.99}$$

and finally for an optimizer

$$\|\partial A\|^2 \le C\kappa\bar{\mu}^2h. \tag{27.2.100}$$

Here μ and $\bar{\mu}$ were calculated for A, but it does not really matter since due to the estimate $|\partial^2 A| \le C\kappa^2h^{-\delta}$ we conclude that $|\partial A - \partial A_\varepsilon| \le C\kappa^2h^{-\delta}\varepsilon \le C$ due to restriction to κ.

Then, for $d=3$

$$\mu^2\bigl(\mu/(\kappa\bar{\mu}|\log h|)\bigr)^3 \le \kappa\bar{\mu}^2h \tag{27.2.101}$$

and if $\mu \geq 1$ we have $\bar{\mu} = \mu$ and (27.2.101) becomes $\kappa^{-3}|\log h|^{-3} \leq C\kappa h$ which is impossible under (27.2.95).

So, $\mu \leq 1$ and (27.2.101) implies (27.2.86) and (27.2.100), (27.2.101) imply that for an optimizer $\|\partial A\| \leq C(\kappa h)^{\frac{1}{2}}$ and $\mu \leq C\kappa^4 h|\log h|^d$. So Statement (i) is proven.

(ii) Proof of Statement (ii) follows then in virtue of arguments of Subsection 27.2.2.

(iii) If $\kappa^*_h \leq \kappa \leq h^{-1}$ we apply the partition-and-rescaling technique. Then $h \mapsto h' = h\gamma^{-1}$ and $\kappa \mapsto \kappa' = \kappa\gamma$ and to get into the framework of (27.2.95) we need $\gamma = \epsilon\kappa^{-\frac{4}{3}} h^{-\frac{1}{3}}|\log(\kappa h)|^{-1}$, leading to the remainder estimate $Ch^{-1}\gamma^{-2}$, which proves Statement (iii). □

Problem 27.2.31. Repeat arguments of Subsubsections *27.2.1.2. Preliminary Analysis* and *27.2.1.3. Estimates* and of this Subsection for $d \neq 3$. When they hold?

27.3 Global Trace Asymptotics in the Case of Coulomb-Like Singularities

27.3.1 Problem

We consider the same operator (27.1.4) as before in $\mathbb{R}^3$ but now we assume that V has Coulomb-like singularities. Namely let $\mathsf{y}_m \in \mathbb{R}^3$ ($m = 1, \dots, M$, where M is fixed) be singularities ("nuclei"). We assume that

$$V = \sum_{1 \leq m \leq M} \frac{z_m}{|x - \mathsf{y}_m|} + W(x) \tag{27.3.1}$$

where

$$z_m \geq 0, \ \ z_1 + \dots + z_M \asymp 1, \tag{27.3.2}$$

and

$$|D^\alpha W| \leq C_\alpha \sum_{1 \leq m \leq M} z_m \bigl(|x - \mathsf{y}_m| + 1\bigr)^{-1} |x - \mathsf{y}_m|^{-|\alpha|} \qquad \forall \alpha : |\alpha| \leq 2, \tag{27.3.3}$$

but at the first stages we will use some weaker assumptions. Later we assume that $V(x)$ decays at infinity sufficiently fast. Let us define $\mathsf{E}^*)$ and $\mathsf{E}(A)$ by (27.2.2)–(27.2.1). Finally, let $\ell(x)\min_{1\le m\le M}\ell_m(x)$ with $\ell_m(x) := \frac{1}{2}|x-\mathsf{y}_m|$.

In this and next Sections we assume that

(27.3.4) $\kappa\in(0,\kappa^*]$ where $0<\kappa^*$ is a small constant.

For $\kappa=0$ we set $A=0$ and consider $\mathsf{E} := \mathsf{Tr}^-(H_{A,V})$; then our results are covered by Chapter 25.

27.3.2 Estimates to a Minimizer

Let us consider a Hamiltonian with potential V and let A be a magnetic potential, minimizing expression (27.2.2). We say that A is a *minimizer* and in the framework of our problems we will prove it existence.

Preliminary Analysis

First, we start from the roughest possible estimate:

Proposition 27.3.1. *Let V satisfy* (27.3.1)–(27.3.3) *and let $\kappa\le\kappa^*$. Then the near-minimizer A satisfies*

$$|\int\bigl(\mathsf{tr}\, e_{A,1}(x,x,0)-\mathsf{Weyl}_1(x)\bigr)\,dx|\le Ch^{-2} \tag{27.3.5}$$

and

$$\|\partial A\|\le C\kappa^{\frac{1}{2}}. \tag{27.3.6}$$

Proof. Definitely (27.3.5)–(27.3.6) follow from the results of L. Erdös, S. Fournais, and J. P. Solovej [3] but we give an independent easier proof, based on our Subsection 27.2.1.

(a) First, let us pick up $A=0$ and consider $\mathsf{Tr}\bigl(\psi_\ell\theta(-H)\psi_\ell\bigr)$ with cut-offs $\psi_\ell(x)=\psi((x-\mathsf{y}_m)/\ell)$ where $\psi\in\mathscr{C}_0^\infty(B(0,1))$ and equals 1 in $B(0,\frac{1}{2})$. Here and below $\theta(\tau-H_{A,V})$ is a spectral projector of H.

Then

$$|\mathsf{Tr}\bigl(\psi_\ell H^-_{A,V}(0)\psi_\ell\bigr)|\le Ch^{-2}\qquad \text{for}\ \ \ell=\ell_*:=h^2. \tag{27.3.7}$$

On the other hand, contribution of $B(x,\ell)$ with $\ell(x)\ge \ell_*$ to the Weyl error does not exceed $C\zeta^2\hbar^{-1}=C\zeta^3\ell h^{-1}$ where $\hbar=h/(\zeta\ell)$ in the rescaling; so after summation over $\ell\ge\ell_*$ we also get $O(h^{-2})$ provided $\zeta^2\le C\ell^{-1}$. Therefore we arrive to the following rather easy inequality:

$$|\int \bigl(\operatorname{tr} e_{0,1}(x,x,0)-\mathsf{Weyl}_1(x)\bigr)\,dx|\le Ch^{-2}. \tag{27.3.8}$$

This is what the rescaling method gives us without careful the study of the singularity.

(b) On the other hand, consider $A\ne 0$. Let us prove first that

$$\operatorname{Tr}^-(\psi_\ell H\psi_\ell)\ge -Ch^{-2}-Ch^{-2}\int |\partial A|^2\,dx \qquad \text{for}\ \ \ell=\ell_*. \tag{27.3.9}$$

Rescaling $x\mapsto (x-\mathsf{y}_m)/\ell$ and $\tau\mapsto\tau/\ell$ and therefore $h\mapsto h\ell^{-\frac{1}{2}}\asymp 1$ and $A\mapsto A\ell^{\frac{1}{2}}$ (because the singularity is Coulomb-like), we arrive to the same problem with the same κ (in contrast to Subsection 27.2.4 where $\kappa\mapsto\kappa\ell$ because of the different scale in τ and h) and with $\ell=h=1$.

In this case the required estimate follows from L. Erdös, J. P. Solovej [1] (we reproduce Lemma 2.1 of this paper in Appendix 27.A.1.

(c) Consider now function ψ_ℓ as in (c) with $\ell\ge\ell_*$. Then according to Theorem 27.2.29 rescaled

$$\begin{gathered}\operatorname{Tr}^-\bigl(\psi_\ell H_{A,V}\psi_\ell\bigr)-\int \mathsf{Weyl}_1(x)\psi_\ell^2(x)\,dx\\ \ge -C\zeta^3\ell h^{-1}-Ch^{-2}\int_{B(x,2\ell/3)}|\partial A|^2\,dx.\end{gathered} \tag{27.3.10}$$

Really, rescaling of the first part is a standard one and in the second part we should have in the front of the integral a coefficient $\kappa^{-1}h^{-2}\zeta^2\times\zeta^{-2}\ell(h/\zeta\ell)^{-2}$ where factor ζ^2 comes from the scaling of the spectral parameter, factor ζ^{-2} comes from the scaling of the magnitude of A, factor $\ell=\ell^3\times\ell^{-2}$ comes from the scaling of dx and ∂ respectively, and $\hbar:=h/(\zeta\ell)$ is a semiclassical parameter after rescaling. Therefore this expression acquires a factor $\zeta^2\ell\le C$.

Then we conclude that

$$\int\bigl(\operatorname{tr} e_{A,1}(x,x,0)-\mathsf{Weyl}_1(x)\bigr)\,dx\ge -Ch^{-2}-Ch^{-2}\int|\partial A|^2\,dx \tag{27.3.11}$$

and adding the magnetic field energy $\kappa^{-1}h^{-2}\|\partial A\|^2$ we find out that

$$\mathsf{E}(A) - \int \mathsf{Weyl}_1(x)\,dx \geq \mathsf{E}(0) - \int \mathsf{Weyl}_1(x)\,dx + (\kappa^{-1} - C)h^{-2}\|\partial A\|^2 - Ch^{-2} \tag{27.3.12}$$

since $\mathsf{Weyl}_1(x)$ does not depend on A. However due to (a) the right-hand expression is greater than $(\kappa^{-1} - C)h^{-2}\|\partial A\|^2 - Ch^{-2}$.

On the other hand, since A is supposed to be a near-minimizer, the left-hand expression of (27.3.12) should not exceed the same expression for $A = 0$ plus Ch^2, i.e. Ch^2 due to (a) again. Then due to)(27.3.4) we arrive to (27.3.5) and (27.3.6). □

Proposition 27.3.2. *Let V satisfy* (27.3.1)–(27.3.3). *Then there exists a minimizer A.*

Proof. After Proposition 27.3.1 has been proven we just repeat arguments of the proof of Proposition 27.2.2. If $V \in \mathscr{L}^{\frac{5}{2}}$ no change would be required but for $V \notin \mathscr{L}^{\frac{5}{2}}$ one needs to consider modifications as in Remark 27.3.3 below. □

Remark 27.3.3. We are a bit ambivalent about a convergence of $\int \mathsf{Weyl}_1(x)\,dx$ at infinity, since for the Coulomb potential it diverges. To avoid this issue, however, we can <u>either</u> assume in addition that $V \in \mathscr{L}^{\frac{5}{2}}$, <u>or</u> tackle it as in Proposition 27.3.16 below.

Estimates to a Minimizer. I

Let us repeat arguments of Subsubsection *27.2.1.3. Estimates.* However our task now is much more complicated: while we know a priory that $\|\partial A\|^2 \leq C\kappa$ we will not be able to improve it significantly (or at all for $\kappa \asymp 1$).

Recall equation (27.2.14) for a minimizer A. After rescaling $x \mapsto x/\ell$, $\tau \mapsto \tau/\zeta^2$, $h \mapsto \hbar = h/(\zeta\ell)$, $A \mapsto A\zeta^{-1}\ell$ this equation becomes

$$\Delta A_j = -2\kappa\zeta^2\ell\hbar^2 \operatorname{Re}\operatorname{tr}\Big[\sigma_j\Big((\hbar Dk - \zeta^{-1}A)_x\cdot\boldsymbol{\sigma} e(x,y,\tau) + e(x,y,\tau)\,{}^t(\hbar D - \zeta^{-1}A)_y\cdot\boldsymbol{\sigma}\Big)\Big]\Big|_{y=x} \tag{27.3.13}$$

and since so far $\zeta^2\ell = 1$ we arrive to

$$\Delta A_j = -2\kappa\hbar^2 \operatorname{Re}\operatorname{tr}\Bigl[\sigma_j\Bigl((\hbar D-\zeta^{-1}A)_x\cdot\boldsymbol{\sigma} e(x,y,\tau)+e(x,y,\tau)\,{}^t(\hbar D-\zeta^{-1}A)_y\cdot\boldsymbol{\sigma}\Bigr)\Bigr]\Bigr|_{y=x}. \tag{27.3.14}$$

(a) Plugging $u=\psi\theta(-H)f$ with cut-off function ψ and repeating arguments of Subsubsection *27.2.1.3. Estimates*, we conclude that in the rescaled coordinates

$$\begin{aligned}\|(\hbar D_x\cdot\boldsymbol{\sigma})u\| &\le \|((\hbar D_x-A)\cdot\boldsymbol{\sigma})u\| + C\|A\|_{\mathscr{L}^6}\cdot\|u\|_{\mathscr{L}^3}\\ &\le \|((\hbar D_x-A)\cdot\boldsymbol{\sigma})u\| + C\hbar^{-\frac12}\|A\|_{\mathscr{L}^6}\cdot\|u\|^{\frac12}\cdot\|\hbar D_x u\|^{\frac12}\\ &\le \|((\hbar D_x-A)\cdot\boldsymbol{\sigma})u\| + \frac12\|\hbar D_x u\| + C(\hbar^{-\frac12}\|A\|_{\mathscr{L}^6})^2\|u\|,\end{aligned} \tag{27.3.15}$$

where $\|A\|_{\mathscr{L}^6}$ calculated in the rescaled coordinates is equal to $\|A_{\mathsf{orig}}\|_{\mathscr{L}^6,\mathsf{orig}}$ (where subscripts "orig"means that the norm is calculated in the original coordinates and A) which does not exceed $C\kappa^{\frac12}$ due to (27.3.6)[12] and therefore (since $\|(\hbar D_x\cdot\boldsymbol{\sigma})u\| = \|\hbar D_x u\|$)

$$\|\hbar D_x u\| \le C\bigl(1+\kappa\hbar^{-1}\bigr)\|f\|. \tag{27.3.16}$$

Continuing arguments of Subsubsection *27.2.1.3. Estimates*, we conclude that in the rescaled coordinates

$$\|(\hbar D_x)^k u\| \le C\bigl(1+\kappa\hbar^{-1}\bigr)^k\|f\|, \tag{27.3.17}$$

$$\|(\hbar D_x)^k((\hbar D_x-A)\cdot\boldsymbol{\sigma})u\| \le C(1+\kappa\hbar^{-1})^k\|f\|, \tag{27.3.18}$$

for $k=0,1,2$ and therefore

$$\|\Delta A\|_{\mathscr{L}^\infty(B(x,1))} \le C\kappa\hbar^{-1}(1+\kappa\hbar^{-1})^3. \tag{27.3.19}$$

Here we estimate different norms of A locally. Then <u>either</u>

$$\|\partial A\|_{\mathscr{L}^\infty(B(x,\frac34))} + \hbar^\delta\|\partial^2 A\|_{\mathscr{L}^\infty(B(x,\frac34))} \le C\kappa\hbar^{-1}(1+\kappa\hbar^{-1})^3 \tag{27.3.20}$$

<u>or</u>

$$\|\partial A\|_{\mathscr{L}^\infty(B(x,1-\epsilon))} + \hbar^\delta\|\partial^2 A\|_{\mathscr{L}^\infty(B(x,1-\epsilon))} \le C\|\partial A\| = C\|\partial A_{\mathsf{orig}}\|_{\mathsf{orig}} \le C\kappa^{\frac12} \tag{27.3.21}$$

[12] As usual we assume that the average of A over $B(x,1)$ is 0.

In the latter case (27.3.21) we have in the original coordinates

$$\|\partial A\|_{\mathscr{L}^\infty(B(x,\ell))} \le C\kappa^{\frac{1}{2}}\ell^{-\frac{3}{2}} \tag{27.3.22}$$

and we are rather happy because then the effective intensity of the magnetic field in $B(x,\ell)$ is $\zeta^{-1}\ell\|\partial A\|_{\mathscr{L}^\infty(B(x,1-\epsilon))}\le C\kappa^{\frac{1}{2}}$.

(b) The former case (27.3.20) is much more complicated because our estimate is really poor for $\kappa\asymp 1$ and we are going to act only in the assumption (27.3.4). Assume that

$$\|\partial A\|_{\mathscr{L}^\infty(B(x,1-\epsilon))} \le \mu \tag{27.3.23}$$

with $\mu\ge\hbar^{-\sigma}$. Selecting $u=\psi\theta(-H)f$ with γ-admissible ψ we conclude that $\|(A\cdot\boldsymbol{\sigma})u\|\le\|A\|_{\mathscr{L}^\infty}\|u\|\le C\mu\gamma\|u\|$ (assuming without any loss of the generality that $A=0$ at some point of $\mathsf{supp}(\psi)$) and that

$$\|(\hbar D)^k u\|\le C(1+\hbar\gamma^{-1}+\mu\gamma)^k,$$
$$\|(\hbar D)^k((\hbar D-A)\cdot\boldsymbol{\sigma})u\|\le C(1+\hbar\gamma^{-1}+\mu\gamma)^{k+1},$$

and therefore

$$|\Gamma_x(\hbar D_x-A)\cdot\boldsymbol{\sigma})e(.,.,0)|\le C\hbar^{-3}(1+\hbar\gamma^{-1}+\mu\gamma)^{\frac{7}{2}},$$

and then

$$\|\Delta A\|_{\mathscr{L}^\infty(B(x,1-\epsilon))}\le C\hbar^{-1}(1+\hbar\gamma^{-1}+\mu\gamma)^{\frac{7}{2}}.$$

Optimizing with respect to $\gamma=\mu^{-\frac{1}{2}}h^{\frac{1}{2}}$ we conclude that <u>either</u>

$$\|\partial^2 A\|_{\mathscr{L}^\infty(B(x,1-\epsilon))}\le C\hbar^{-1-\delta}(1+\hbar\mu)^{\frac{7}{4}} \tag{27.3.24}$$

<u>or</u> (27.2.21) holds. In the former case of (27.3.24), using the second of estimates

$$\|A\|_{\mathscr{L}^\infty(B(x,1-\epsilon))}\le C\|\partial^2 A\|^{\frac{1}{5}}_{\mathscr{L}^\infty(B(x,1-\epsilon))}\|\partial A\|^{\frac{4}{5}}, \tag{27.3.25}$$

$$\|\partial A\|_{\mathscr{L}^\infty(B(x,1-\epsilon))}\le C\|\partial^2 A\|^{\frac{3}{5}}_{\mathscr{L}^\infty(B(x,1-\epsilon))}\|\partial A\|^{\frac{2}{5}} \tag{27.3.26}$$

we conclude that (27.3.23) holds with $\mu=\mu'$,

$$\mu' \coloneqq \hbar^{-\frac{3}{5}-\delta}(1+\hbar\mu)^{\frac{21}{20}}$$

and one can see easily that starting from $\mu=\hbar^{-4}$ as given by (27.3.20), we can arrive after number of iterations to $\mu=\hbar^{-\frac{3}{5}-\delta}$ and therefore

$$\|\partial^k A\|_{\mathscr{L}^\infty(B(x,1-\epsilon))}\le C\hbar^{-\frac{1}{5}(1+2k)-\delta}\qquad k=0,1,2. \tag{27.3.27}$$

(c) This estimate (27.3.27) is good enough to launch our microlocal arguments. Assuming (27.3.23) with $\mu \le h^{\sigma-1}$ we estimate as in Section 27.2

$$|\Gamma_x((\hbar D_x - A)\cdot \boldsymbol{\sigma})e(.,.,0)| \le C\mu\hbar^{-\delta},$$

and then

$$\|\partial^2 A\|_{B(x,1-\epsilon)} \le C\mu h^{-\delta},$$

and therefore

$$\|\partial A\|_{B(x,1-\epsilon)} \le C\mu^{\frac{3}{5}}h^{-\delta},$$

resulting in $\mu := \mu^{\frac{3}{5}}h^{-\delta}$ and after a number of iterations we get $\mu = h^{-\delta}$, and therefore iterating this procedure one more time and taking into account factor κ we arrive to

(27.3.28) Either (27.3.21) holds or

$$\|\partial^2 A\|_{\mathscr{L}^\infty(B(x,1-\epsilon))} \le C\kappa h^{-\delta}. \tag{27.3.29}$$

However to prove that the effective magnetic field is $O(1)$ we need to modify these arguments, and we do it in the next subsubsection.

Estimates to a Minimizer. II

In this step we repeat arguments of Subsubsection *27.2.2.1. Sharp Estimates*, but now we have a problem: we cannot use $\mu = \|\partial A\|_\infty$ since we have domains $\mathcal{X}_r = \{x : \ell(x) \ge r\}$ rather than the whole space. So we get the following analogue of (27.2.48) where A is still rescaled and the norms are calculated in the rescaled coordinates:

$$\|\Delta A\|_{\mathscr{C}(B(x,\frac{3}{4})} + \hbar\|\Delta\partial A\|_{\mathscr{C}(B(x,\frac{3}{4})} \le \\ C\kappa\Bigl(1 + |\partial A|_{\mathscr{C}(B(x,1)} + h^{\frac{1}{2}(\theta-1)}\|\partial A\|_{\mathscr{C}^{\theta\frac{1}{2}}(B(x,1)}\Bigr), \tag{27.3.30}$$

which implies

$$\|\partial A\|_{\mathscr{C}(B(x,\frac{1}{2}))} + \hbar^{\theta-1}\|\partial A\|_{\mathscr{C}^\theta(B,(x,\frac{1}{2}))} \le \\ \epsilon\hbar^{(\theta-1)}\zeta^{-1}\|\partial A\|_{\mathscr{C}^\theta(B(x,1))} + C\kappa\|\partial A\|_{\mathscr{C}(B(x,1))} + C\|\partial A\|_{\mathscr{L}^2(B(x,1))} \tag{27.3.31}$$

and the last term in the right-hand expression does not exceed $C\kappa^{\frac{1}{2}}$.

Let $\nu(r)=\sup_{x:\,\ell(x)\ge r} f(x)$, where $f(x)$ is the left-hand expression of (27.3.16), calculated for given x in the rescaled coordinates. Then (27.3.31) implies that for $\kappa\in(0,\kappa^*)$ (where $\kappa^*>0$ is a small constant)

$$\nu(r)\le \frac{1}{2}\nu(\frac{1}{2}r)+C\kappa^{\frac{1}{2}},$$

which in turn implies that

$$\nu(r)\le \frac{1}{2}\nu(2^{-n}r)+2C\kappa^{\frac{1}{2}},\qquad n\ge 1,$$

and therefore

$$\nu(r)\le 4C\kappa^{\frac{1}{2}}+4\sup_{C_0h^2\le\ell(x)\le 2C_0h^2} f(x)\le C_1\kappa^{\frac{1}{2}}$$

due to the rough estimate (because $\hbar\asymp 1$ for $\ell(x)\asymp h^2$). Then returning to the original (not rescaled) coordinates and to the original (not rescaled) potential A we arrive to estimates (27.3.32) and (27.3.33) below:

Proposition 27.3.4. *Let $\kappa\le\kappa^*$, $\zeta=c\ell^{-\frac{1}{2}}$. Let A be a minimizer. Then for $\ell(x)\ge\ell_*=h^2$ estimate* (27.3.22) *holds and also*

$$|\partial^2A(x)-\partial^2A(y)|\le C\kappa^{\frac{1}{2}}\ell^{-\frac{5}{2}}|x-y|^\theta\ell^{\theta/2}\ell_*^{-\theta/2}\qquad 0<\theta<1, \tag{27.3.32}$$

and

$$|\partial A(x)-\partial A(y)|\le C\kappa^{\frac{1}{2}}\ell^{-\frac{5}{2}}|x-y|(1+|\log|x-y||). \tag{27.3.33}$$

Remark 27.3.5. (i) So far we used only assumption that

$$|\partial^\alpha V|\le C\zeta^2\ell^{-|\alpha|}\qquad\forall\alpha:|\alpha|\le 2 \tag{27.3.34}$$

with $\zeta=\ell^{-\frac{1}{2}}$ but even this was excessive.

(ii) In this framework however we cannot prove better estimates because (27.3.22) always remains a valid alternative even if $\zeta\ll\ell^{-\frac{1}{2}}$.

(iii) Originally we need an assumption (27.2.37) $|V|\ge\epsilon_0$, but for $d=3$ one can easily get rid of it by the standard rescaling technique.

Consider now zone $\{x:\ \ell(x)\le\ell_*\}$:

Proposition 27.3.6. *Let $\kappa\le\kappa^*$, $\zeta\le c\ell^{-\frac{1}{2}}$. Let A be a minimizer. Then $|\partial A|\le C\kappa^{\frac{1}{2}}h^{-3}$ for $\ell(x)\le\ell_*=h^2$.*

Proof. Proof is standard, based on the rescaling (then $\hbar = 1$) and equation (27.2.14) for a minimizer A. We leave easy details to the reader. □

Let us slightly improve estimate to a minimizer A. We already know that $|\partial A(x)| \le C_0\beta$ with $\beta = \ell^{-\frac{3}{2}}$ and using the standard rescaling technique we conclude that

$$|\Delta A| \le C\kappa\zeta^2\beta + C\kappa\zeta^3\ell^{-1}, \tag{27.3.35}$$

which does not exceed $C\kappa\ell^{-\frac{5}{2}}$ which implies

Proposition 27.3.7. *In our framework*

(i) If $\ell(x) \ge \ell_* := h^2$, then

$$|A| \le C\kappa\ell^{-\frac{1}{2}}, \qquad |\partial A| \le C\kappa\ell^{-\frac{3}{2}} \tag{27.3.36}$$

and

$$|\partial A(x) - \partial A(y)| \le C_\theta\kappa\ell^{-\frac{3}{2}-\theta}|x-y|^\theta \qquad \text{as } |x-y| \le \frac{1}{2}\ell(x) \tag{27.3.37}$$

for any $\theta \in (0,1)$.

(ii) If $\ell(x) \le \ell_*$, then these estimates hold with $\ell(x)$ replaced by ℓ_*.

Remark 27.3.8. (i) Here in comparison with old estimates we replaced factor $\kappa^{\frac{1}{2}}$ by κ which is an advantage.

(ii) These estimates imply that $\int_{\{x:\, \ell(x)\le 1\}} |\partial A|^2\, dx \le C\kappa^2|\log h|$ while in fact it must not exceed $C\kappa$.

Estimates to a Minimizer. III

Consider now external zone $\mathcal{Y} := \{x\colon \ell(x) \ge 1\}$ and assume that

$$\zeta(x) \le C\ell(x)^{-\nu} \qquad \text{for } \ell(x) \ge 1 \tag{27.3.38}$$

with $\nu > 1$.

Then if also $|\partial A(x)| = O(\ell(x)^{-\nu_1})$ for $\ell(x) \ge 1$ then the right hand expression of (27.3.35) does not exceed $C\kappa(\ell^{-3\nu-1} + \ell^{-\nu_1-2\nu})$ and therefore we *almost* upgrade estimate for $|\partial A(x)|$ to $O(\ell^{-3\nu} + \ell^{-\nu_1-2\nu+1})$ and repeating these arguments sufficiently many times to $O(\ell^{-3\nu})$.

However, there are several obstacles to this conclusion: first, if $\nu > 1$ we conclude that

$$A_j = \sum_m \alpha_{j,m} |x - \mathsf{y}_m|^{-1} + O(\ell^{-1-\delta})$$

with constant $\alpha_{j,m}$; however assumption $\nabla \cdot A = 0$ implies $\alpha_{j,m} = 0$ and we pass this obstacle.

Indeed, let our equation be $\Delta A_j = \Phi_j$ and therefore

$$A_j(x) = -\frac{1}{4\pi} \int |x - y|^{-1} \Phi_j(y)\, dy.$$

Let a be the minimal distance between nuclei, $1 = \sum_{0\le m\le M} \phi_m$ where ϕ_m is supported in $\frac{1}{3}a$-vicinity of y_m and equals 1 in $\frac{1}{4}a$-vicinity of y_m, $m = 1, \dots, 1$. Let

$$I_{j,m} = \int \Phi_j(y)\phi_m(y)\, dy, \qquad \eta = \max_{1\le m\le M} |I_{j,m}|.$$

Then if x belongs to b-vicinity of y_m with $b \le \epsilon a$ one can prove easily that

$$|\partial_{x_k} \int |x - y|^{-1} \Phi_j(y)\phi_{m'}(y)\, dy| \le C\eta a^{-2} + Ca^{-3}$$

for $m' = 0, 1, \dots, M$, $m' \ne m$.

Also one can prove easily that

$$|\partial_{x_j} \Bigl(\int |x - y|^{-1} \Phi_j(y)\phi_{m'}(y)\, dy - |x - \mathsf{y}_m|^{-1} I_{j,m} \Bigr)| \le C|x - \mathsf{y}_m|^{-3},$$

and combining with the previous inequality and with equation $\nabla \cdot A = 0$ we conclude that $|I_{m,j}| \le C\eta a^{-2} b^2 + Ca^{-3} b^2 + Cb^{-1}$ for $b \le \epsilon a$. Then selecting $b = \epsilon_1 a$ with sufficiently small constant ϵ_1, we conclude that $\eta \le Ca^{-1}$ which in turn implies that $|\partial_k A_j(x)| \le C\ell^{-3}$.

The second obstacle

$$A_j = \sum_{k,m} \alpha_{jk,m} (x_k - \mathsf{y}_{k,m}) |x - \mathsf{y}_m|^{-3} + O(\ell^{-2})$$

with constant $\alpha_{jk,m}$ we cannot pass since assumption $\nabla \cdot A = 0$ implies only that modulo gradient $A = \sum_m \beta_m \times \nabla \ell_m^{-1}$ with constant vectors β_m and one cannot do anything about this.

Therefore we upgrade (27.3.36)–(27.3.37) there:

Proposition 27.3.9. *In our framework assume additionally that* (27.3.38) *holds. Then for* $\nu > \frac{4}{3}$

$$|A| \le C\kappa\ell^{-2}, \qquad |\partial A| \le C\kappa\ell^{-3} \tag{27.3.39}$$

and

$$|\partial A(x) - \partial A(y)| \le C_\theta \kappa \ell^{-3-\theta}|x-y|^\theta \qquad \textit{as}\ \ |x-y| \le \frac{1}{2}\ell(x) \tag{27.3.40}$$

if $\ell(x) \ge 1$ *(for all* $\theta \in (0,1)$*).*

Remark 27.3.10. (i) In application to the ground state energy we are interested in $\nu = 2$.

(ii) Observe that for $a \ge 1$

$$\int_{\{\ell(x)\asymp a\}} |\partial A|^2\, dx = O(\kappa^2 a^{-3}). \tag{27.3.41}$$

(iii) We were not able to improve (27.3.39)–(27.3.41) no matter how fast ζ decays.

27.3.3 Basic Trace Estimates

Recall that the standard Tauberian theory results in the remainder estimate $O(h^{-2})$. Indeed, since the effective magnetic field intensity is no more than $C\kappa$, the contribution of $B(x,\ell(x))$ to the Tauberian error[13)] does not exceed $C\zeta^2 \times \hbar^{-1} = C\zeta^3\ell h^{-1}$, which for $\zeta \asymp \ell^{-\frac{1}{2}}$ translates into $C\ell^{-\frac{1}{2}}h^{-1}$ and summation over domain $\{x : \ell(x) \ge \ell_* = h^2\}$ results in Ch^{-2}. On the other hand, contribution of the domain $\{x : \ell(x) \le \ell_* = h^2\}$ into asymptotics does not exceed $C\hbar^{-3}\ell_*^{-1} = Ch^{-2}$ for $\hbar = 1$.

However, now we can unleash arguments of V. Ivrii and I. M. Sigal [1]. Recall that we are looking at

$$\mathsf{Tr}(\psi H^-_{A,V}\psi) = \mathsf{Tr}(\phi_1 H^-_{A,V}\phi_1) + \mathsf{Tr}(\phi_2 H^-_{A,V}\phi_2) \tag{27.3.42}$$

where $\psi^2 = \phi_1^2 + \phi_2^2$, $\mathsf{supp}(\phi_1) \subset \{x, |x| \le 2r\}$, $\mathsf{supp}(\phi_2) \subset \{x, r \le |x| \le b\}$ and we compare it with the same expression calculated for H_{A,V^0} with $V^0 = Z_m|x|^{-1}$. Here we assume that

$$a \le 1, \qquad z \asymp 1 \tag{27.3.43}$$

13) And then to the Weyl error because we will explain transition from the Tauberian to Weyl estimates below.

and

$$|D^\alpha(V-V^0)|\le c_0 a^{-1}\ell^{-|\alpha|}\qquad \forall\alpha:|\alpha|\le 3. \tag{27.3.44}$$

The latter assumption is too restrictive and could be weaken. Then if $\phi(x)$ is an ℓ-admissible partition element

$$\operatorname{Tr}\bigl(\theta(-H^-_{A,V})\phi^2\bigr)=\int \mathsf{Weyl}(x)\phi^2(x)\,dx+O(rh^{-2}) \tag{27.3.45}$$

and

$$\operatorname{Tr}\bigl(H^-_{A,V}\phi^2\bigr)=\int \mathsf{Weyl}_1(x)\phi^2(x)\,dx+O(r^{-\frac{1}{2}}h^{-1}), \tag{27.3.46}$$

where the error estimates are $O(\hbar^{-2})$ and $O(\zeta^2\hbar^{-1})$ respectively. One can justify transition from the Tauberian to Weyl errors by considering Tauberian expressions and considering $H_{A_\varepsilon,V}$ and $H_{A,V}$ as unperturbed and perturbed operators respectively; their difference is $O(\zeta^3\varepsilon^2)$ with $\varepsilon=\hbar^{1-\delta}$.

Then the contribution[14)] of the time interval $\{t\colon t\asymp T\}$ to the Tauberian expression for (27.3.45) of the first term in the approximation does not exceed $C\hbar^{-4}T\times(\hbar T^{-1})^s$, of the second term $C\hbar^{-4}T\times(\hbar T^{-1})^sT\hbar^{-1}\varepsilon^2$, and of the third term $C\hbar^{-4}T\times(\hbar T^{-1})T^2\hbar^{-2}\varepsilon^4$. One can see easily that the end of the day the first term gives us the Weyl expression, the second term turns out to be 0, and the third term is less than the announced error.

Similarly, the contribution[14)] of the time interval $\{t\colon t\asymp T\}$ to the Tauberian expression for (27.3.46) of the first term in the approximation does not exceed $C\zeta^2\hbar^{-4}T\times(\hbar T^{-1})^s$, of the second term $C\zeta^2\hbar^{-4}T\times(\hbar T^{-1})^sT\hbar^{-1}\varepsilon^2$ and of the third term $C\hbar^{-4}T\times(\hbar T^{-1})^2T^2\hbar^{-2}\varepsilon^4$. Again, in the end of the day the first tem gives us the Weyl expression, the second term turns out to be 0, and the third term is less than the announced error.

The same estimates also hold for operator H_{A,V^0} and then using ℓ-admissible partition of unity we conclude that

$$\operatorname{Tr}\bigl(\phi_2(H^-_{A,V}-H^-_{A,V^0})\phi_2\bigr)=\\ \int\bigl(\mathsf{Weyl}_1(x)-\mathsf{Weyl}_1^0(x)\bigr)\,\phi_2^2(x)\,dx+O(r^{-\frac{1}{2}}h^{-1}), \tag{27.3.47}$$

where Weyl_1^0 and Weyl^0 are calculated for operator with potential V^0. Indeed, we just proved this for each operator $H_{A,V}$ and H_{A,V^0} separately.

14) After standard rescaling $x\mapsto x\ell^{-1}$, $\xi\mapsto\xi\zeta^{-1}$, $h\mapsto\hbar$, $\tau\mapsto\tau\zeta^{-2}$, and $t\mapsto t\zeta\ell^{-1}$.

On the other hand, considering $V^\eta = V^0(1-\eta) + V\eta = V^0 + W\eta$ and following V. Ivrii and I. M. Sigal [1], we can rewrite the similar expression albeit for $\phi_2 = 1$ as

$$\operatorname{Tr}\Bigl(\int_0^1 W\theta(-H_{A,V^\eta})\,d\eta\Bigr) \tag{27.3.48}$$

and applying the semiclassical approximation (under the temporary assumption that W is supported in the domain $\{x:\ |x|\le 4r\}$) one can prove that for $\phi_1 = 1$

$$\operatorname{Tr}\bigl(\phi_1(H^-_{A,V} - H^-_{A,V^0})\phi_1\bigr) = \int \bigl(\mathsf{Weyl}_1(x) - \mathsf{Weyl}^0_1(x)\bigr)\,\phi_1^2(x)\,dx + O(a^{-1}rh^{-2}). \tag{27.3.49}$$

Really, due to (27.3.45) and (27.3.44) the contribution of the ball $B(x,\ell(x))$ does not exceed $Ca^{-1}\hbar^{-2} = Ca^{-1}\ell(x)h^{-2}$ and summation with respect to partition with $\ell(x)\le 4r$ returns $Ca^{-1}rh^{-2}$); meanwhile, the contribution of $\{x:\ell(x)\le \ell_*\}$ does not exceed $Ca^{-1}\hbar^{-2} = Ca^{-1}$ since there $\hbar = 1$.

One can get easily rid of the temporary assumption and take ϕ_1 supported in $\{x:\ell(x)\le 2r\}$ instead.

Therefore we arrive to

Proposition 27.3.11. *Under assumption* (27.3.44)

$$\operatorname{Tr}\bigl(\psi(H^-_{A,V} - H^-_{A,V^0})\psi\bigr) = \int \bigl(\mathsf{Weyl}_1(x) - \mathsf{Weyl}^0_1(x)\bigr)\,\psi^2(x)\,dx + O\bigl(a^{-\frac{1}{3}}h^{-\frac{4}{3}}\bigr). \tag{27.3.50}$$

Really, $a^{-\frac{1}{3}}h^{-\frac{4}{3}}$ is $r^{-\frac{1}{2}}h^{-1} + a^{-1}rh^{-2}$ optimized by $r\asymp r_* \coloneqq (ah)^{\frac{2}{3}}$; since $h^2\le a$ we note that $h^2\le r_*\le a$.

Corollary 27.3.12. *(i) For $M=1$ equality* (27.3.50) *remains valid with $\psi = 1$ and $a=1$.*

(ii) For $M\ge 2$ and $a\ge h^2$ equality (27.3.50) *becomes*

$$\operatorname{Tr}\bigl(\psi(H^-_{A,V} - H^-_{A,V^0})\psi\bigr) = \int \bigl(\mathsf{Weyl}_1(x) - \mathsf{Weyl}^0_1(x)\bigr)\,\psi^2(x)\,dx + O\bigl((a^{-\frac{1}{3}}+1)h^{-\frac{4}{3}}\bigr), \tag{27.3.51}$$

where we reset case $a\ge 1$ to $a=1$.

27.3.4 Improved Trace Estimates

Improved Tauberian Estimates

Let us apply much more advanced arguments of Section 12.6; recall that these arguments are using the long term propagation of singularities. Unfortunately, using these arguments, we are not able to improve the above results unless $\kappa \ll 1$.

First, let us consider ψ, which is r-admissible partition element located in $\{x : \ell(x) \asymp r\}$, and we need to estimate an absolute value of

$$F_{t\to h^{-1}\tau}\bar{\chi}_T(t)\operatorname{Tr}\bigl(e^{ih^{-1}tH}\psi\bigr), \tag{27.3.52}$$

and to do it we need to estimate the same expression with $\bar{\chi}_T(t)$ replaced by $\chi_{T'}(t)$ with $t_0 \le T' \le T$ where $t_0 = \epsilon\ell\zeta^{-1} = \epsilon r^{\frac{3}{2}}$. We can break $\psi = \psi^+ + \psi^-$ with $\psi^\pm = \psi^\pm(x, hD)$ such that the trajectories in the positive (negative) time direction from support of its symbol $\psi^+(x,\xi)$ are going after time Ct_0 in the direction of increased $\ell(x)$, and since we consider the trace we need to consider only ψ^+ and only $\chi \in \mathscr{C}^\infty([\frac{1}{2}, 1])$.

The trouble is that we have not rough but non-smooth magnetic field[15]; so let us consider $t_0 + t_1 + \ldots + t_n \asymp T'$ where $t_j = \epsilon r_j^{\frac{3}{2}}$, $r_j = c^j r$, $j = 0, 1, \ldots, n$, and let us estimate an error appearing when we replace in (modified) (27.3.52) $e^{ih^{-1}tH}\psi^+$ by

$$e^{ih^{-1}(t-t_n)H}\psi^+_{n+1}e^{ih^{-1}t_nH}\psi^+_n\cdots e^{ih^{-1}t_1H}\psi^+_1 e^{ih^{-1}t_0H}\psi^+ \tag{27.3.53}$$

with ψ_j^+ defined similarly and Hamiltonian flow from $\operatorname{supp}(\psi_j^+)$ for $t = t_j$ is inside $\{(x,\xi)\colon \psi^+_{j+1}(x,\xi) = 1\}$. Therefore we need to estimate an error when we insert ψ_j^+.

According to our propagation results (namely, Proposition 27.2.11) after $\psi_1^+, \ldots, \psi_{j-1}^+$ were inserted, insertion of ψ_j^+ brings a relative error not exceeding $C\bigl(\hbar_j^\theta \|\partial A\|_{\theta, Y_j} + \hbar_j^{s+1}\bigr)$, where $\hbar_j = hr_j^{-\frac{1}{2}}$ and Y_j is an ϵr_j-vicinity of the x-projection of $\operatorname{supp}(\psi_j)$; s is an arbitrarily large exponent.

Recall that $\|\partial A\|_{\theta, Y_j} \le C\kappa\hbar_j^{1-\theta}$ for $\theta \in (1,2)$; therefore this relative error does not exceed $C\hbar_j(\kappa + \hbar_j^s)$. Therefore inserting all ψ_j^+ brings a relative error $C\sum_{j\ge 0}\hbar_j(\kappa + \hbar_j^s) \asymp C\hbar(\kappa + \hbar^s)$ and since a priory expression (27.3.52) is bounded by $C\hbar^{-3}T$ we conclude that

[15] More precisely, A is rough but with the roughness parameter $\hbar$ which is a bit too small.

(27.3.54) The absolute value of expression (27.3.52) with $\bar{\chi}_T(t)$ replaced by $\chi_{T'}(t)$ with $T_* \asymp r^{\frac{3}{2}} \le T' \le T^*$ [16] does not exceed $C\hbar^{-2}(\kappa + \hbar^s)T'$.

Then an absolute value of expression (27.3.52) with $\bar{\chi}_T(t)$ replaced by $(\bar{\chi}_T(t) - \bar{\chi}_{T_*})$ does not exceed $C\hbar^{-2}(\kappa + \hbar^s)$ and since expression (27.3.52) with $T = T_*$ does not exceed $C\hbar^{-2}t_0$ we conclude that

(27.3.55) The absolute value of expression (27.3.52) with $T_* \le T \le T^*$ does not exceed $C\hbar^{-2}T_* + C\hbar^{-2}(\kappa + \hbar^s)T$.

Then we conclude that

(27.3.56) An error when we replace $\operatorname{Tr}\bigl(\theta(-H_{A,V})\psi\bigr)$ by its Tauberian expression with "time" T does not exceed $C\hbar^{-2}\bigl(T_*T^{-1} + \kappa + \hbar^s\bigr)$

and

(27.3.57) An error when we replace $\operatorname{Tr}\bigl(H^-_{A,V}\psi\bigr)$ by its Tauberian expression with "time" T does not exceed $C\hbar^{-1}\bigl(T_*T^{-1} + \kappa + \hbar^s\bigr)T_*T^{-1}\zeta^2$.

In the latter statement we need to remember how everything scales.

Observe that presence of the magnetic field due to its estimates relatively perturbs dynamics by $O(\kappa)$ and therefore if κ is sufficiently small (i.e. $\kappa \le \kappa^*$) it does not affect T^*. Then assuming that

$$|\nabla^\alpha(V - V^0)| \le \epsilon a^{-1}r^{-|\alpha|} \qquad \forall\alpha : |\alpha| \le 1, \qquad V^0 = Zr^{-1} \\ \text{with} \quad Z \asymp 1, \quad a \ge h^{2-\delta} \tag{27.3.58}$$

we can take $T^* \asymp a^{\frac{3}{2}}$ and therefore we conclude that the Tauberian error in (27.3.57) does not exceed

$$Ch^{-1}a^{-\frac{3}{2}}r\bigl(r^{\frac{3}{2}}a^{-\frac{3}{2}} + \kappa + h^s r^{-\frac{1}{2}s}\bigr) \tag{27.3.59}$$

and we arrive to Statement (i) in Proposition 27.3.13 below.

Meanwhile, the Tauberian error in $\operatorname{Tr}\bigl((H^-_{A,V} - H^-_{A,V^0})\psi\bigr)$ does not exceed

$$Ca^{-1}h^{-2}r\bigl(r^{\frac{3}{2}}a^{-\frac{3}{2}} + \kappa + h^s r^{-\frac{1}{2}s}\bigr) \tag{27.3.60}$$

and we arrive to Statement (ii) below:

[16] We discuss the choice of T^* later.

Proposition 27.3.13. *Assume that* (27.3.58) *is fulfilled and let* ψ *be* ℓ-*admissible function supported in* $\{x\colon \ell(x)\asymp r\}$ *with* $h^2\le r\le a$. *Let* A *satisfy minimizer estimate. Then*

(i) The Tauberian error with $T=T^*\asymp a^{\frac{3}{2}}$ *in* $\operatorname{Tr}\bigl(H^-_{A,V}\psi\bigr)$ *does not exceed* (27.3.59).

(ii) The Tauberian error with $T=T^*\asymp a^{\frac{3}{2}}$ *in* $\operatorname{Tr}\bigl((H^-_{A,V}-H^-_{A,V^0})\psi\bigr)$ *does not exceed* (27.3.60).

Proof. An easy proof following arguments of Section 12.6 is left to the reader. □

Observe that in the deduction of Statement (i) summation with respect to $r: b\le r\le a$ returns $Ch^{-1}a^{-\frac{1}{2}}$ and in the deduction of (ii) summation with respect to $r: h^2\le r\le b$ returns $Ch^{-2}\bigl(a^{-\frac{5}{2}}b^{\frac{5}{2}}+\kappa a^{-1}b\bigr)+Ca^{-1}$. Note also that Statement (ii) remains true for r-admissible function supported in $\{x\colon \ell(x)\le r\}$ with $r\asymp h^2$. Then we arrive to

Corollary 27.3.14. *Assume that* (27.3.58) *is fulfilled. Then*

(i) Let ϕ_2 *be* ℓ-*admissible function supported in* $\{x\colon b\le \ell(x)\le a\}$. *Then the Tauberian error with* $T=T^*\asymp a^{\frac{3}{2}}$ *in* $\operatorname{Tr}\bigl(H^-_{A,V}\phi_2\bigr)$ *does not exceed* $Ch^{-1}a^{-\frac{1}{2}}$.

(ii) Let ϕ_1 *be* ℓ-*admissible function supported in* $\{x\colon \ell(x)\le b\}$. *Then the Tauberian error with* $T=T^*\asymp a^{\frac{3}{2}}$ *in* $\operatorname{Tr}\bigl((H^-_{A,V}-H^-_{A,V^0})\phi_1\bigr)$ *does not exceed* $Ch^{-2}\bigl(a^{-\frac{5}{2}}b^{\frac{5}{2}}+\kappa a^{-1}b\bigr)+Ca^{-1}$.

Remark 27.3.15. Obviously we do not need any new assumptions on κ to estimate the sum of expressions obtained in Statements (i) and (ii) of Corollary 27.3.14 by $Ch^{-1}a^{-\frac{1}{2}}$ (as $b\le a^{\frac{1}{2}}h$) here but we need to move from Tauberian expression to Weyl expression.

Improved Weyl eEstimates

Note that in virtue of (27.3.54) for element ψ the contribution of the time interval $\{t\colon |t|\asymp T'\}$ to the Tauberian expression for $\operatorname{Tr}\bigl(H^-_{A,V}\psi\bigr)$ does not exceed $C\hbar^{-1}\bigl(\kappa+\hbar^s\bigr)T_*T'^{-1}\zeta^2$, and therefore, replacing $\bar\chi_T(t)$ by $\bar\chi_{T_*}(t)$ we introduce an error not exceeding

$$C\hbar^{-1}\bigl(\kappa+\hbar^s\bigr)\zeta^2\asymp Ch^{-1}r^{-\frac{1}{2}}\bigl(\kappa+h^sr^{-\frac{1}{2}s}\bigr) \tag{27.3.61}$$

and summation with respect to $r: b \le r \le a$ returns

$$Ch^{-1}b^{-\frac{1}{2}}\bigl(\kappa + h^s b^{-\frac{1}{2}s}\bigr). \tag{27.3.62}$$

On the other hand, also in virtue of (27.3.54) for element ψ the contribution of the time interval $\{t\colon |t|\asymp T'\}$ to the Tauberian expression for $\operatorname{Tr}\bigl((H^-_{A,V} - H^-_{A,V^0})\psi\bigr)$ does not exceed $C\hbar^{-2}a^{-1}\bigl(\kappa+\hbar^s\bigr)$, and therefore replacing $\bar\chi_T(t)$ by $\bar\chi_{T_*}(t)$ we introduce an error not exceeding

$$Ch^{-2}a^{-1}r\bigl(\kappa + h^s r^{-\frac{1}{2}s}\bigr)|\log T/T_*|.$$

Further, in virtue of (27.3.55) the Tauberian error does not exceed $Ch^{-2}a^{-1}r\bigl(r^{\frac{3}{2}}T^{-1}+\kappa + h^s r^{-\frac{1}{2}s}\bigr)$, and adding these two errors together and optimizing their sum by $T\le a^{\frac{3}{2}}$ we get $T\asymp r^{\frac{5}{2}}(\kappa + h^s r^{-\frac{1}{2}s})^{-1}$ and the sum

$$Ch^{-2}a^{-1}r\bigl(\kappa + h^s r^{-\frac{1}{2}s}\bigr)\bigl(|\log(\kappa + h^s r^{-\frac{1}{2}s})|+1\bigr) + Ch^{-2}a^{-\frac{5}{2}}r^{\frac{5}{2}}. \tag{27.3.63}$$

Meanwhile repeating arguments of Subsection 27.3.3 one can see easily that

(27.3.64) The difference between the Tauberian expression with $T=T_*$ and the Weyl expression for $\operatorname{Tr}\bigl(H^-_{A,V}\psi\bigr)$ does not exceed (27.3.61) with any $s<2$

and

(27.3.65) The difference between the Tauberian expression with $T=T_*$ and the Weyl expression for $\operatorname{Tr}\bigl((H^-_{A,V} - H^-_{A,V^0})\psi\bigr)$ does not exceed

$$Ch^{-2}a^{-1}r\bigl(\kappa + h^s r^{-\frac{1}{2}s}\bigr) \tag{27.3.66}$$

with any $s<2$ and thus does not exceed (27.3.63).

Summation with respect to $r: h^2\le r\le b$ of (27.3.63) returns

$$Ch^{-2}a^{-1}b\kappa|\log\kappa| + Ch^{-2}b^{\frac{5}{2}}a^{-\frac{5}{2}} + Ca^{-1}; \tag{27.3.67}$$

adding expression (27.3.62) and optimizing the sum by $b\colon h^2\le b\le a$ we get $b\asymp (ah|\log\kappa|)^{\frac{2}{3}}$ and expression

$$Ch^{-\frac{4}{3}}a^{-\frac{1}{3}}\kappa|\log\kappa|^{\frac{1}{3}} + Ch^{-1}a^{-\frac{1}{2}}. \tag{27.3.68}$$

Thus we have proven

Proposition 27.3.16. *(i) In the framework of Proposition 27.3.11*

$$\operatorname{Tr}\bigl(\psi(H^-_{A,V} - H^-_{A,V^0})\psi\bigr) = \int \bigl(\mathsf{Weyl}_1(x) - \mathsf{Weyl}_1^0(x)\bigr)\,\psi^2(x)\,dx + O\bigl(h^{-\frac{4}{3}}a^{-\frac{1}{3}}\kappa|\log\kappa|^{\frac{1}{3}} + h^{-1}a^{-\frac{1}{2}}\bigr). \tag{27.3.69}$$

(ii) In particular, if

$$\kappa \le ca^{-\frac{1}{6}}h^{\frac{1}{3}}|\log ah^{-2}|^{-\frac{1}{3}} \tag{27.3.70}$$

the error in (27.3.69) *does not exceed* $Ch^{-1}a^{-\frac{1}{2}}$ *exactly as in the case without magnetic field.*

Remark 27.3.17. (i) Obviously we could consider $a = 1$ and then just rescale $x \mapsto xa^{-1}$, $\tau \mapsto \tau a$, $h \mapsto ha^{-\frac{1}{2}}$.

(ii) One may wonder if the same approach works for estimate of A. First of all, there is no improvement for estimate for $|\partial^2 A|$ because it follows from the estimate for $|\Delta A|$ which is a pointwise estimate.

(iii) Still, since ∂A and A are mollifications of ΔA one can improve estimates for them if $\kappa \ll 1$ and $\ell \ll a$; however, there are no improvements if either $\kappa \asymp 1$ or $\ell \ge a$. Since these improvements do not lead to the improvements of our final results we do not pursue them.

27.3.5 Single Singularity

Coulomb Potential

Consider now exactly Coulomb potential: $V = Z|x|^{-1}$. Let us establish the existence of the Scott correction:

Proposition 27.3.18. *Let* $V = Z|x|^{-1}$, $h > 0$, $Z > 0$ *and* $0 < \kappa \le \kappa^*$. *Then*

(i) The following limit exists

$$\lim_{r\to\infty}\Bigl(\inf_A\Bigl(\operatorname{Tr}\bigl((\phi_r H_{A,V}\phi_r)^-\bigr) + \frac{1}{\kappa h^2}\int |\partial A|^2\,dx\Bigr) - \int \mathsf{Weyl}_1(x)\phi_r^2(x)\,dx\Bigr) =: 2Z^2h^{-2}S(Z\kappa). \tag{27.3.71}$$

(ii) And it coincides with

$$\lim_{\eta\to 0^+}\Bigl(\inf_{A,V}\Bigl(\mathsf{Tr}\bigl((H_{A,V}+\eta)^-\bigr)\bigr)+\frac{1}{\kappa h^2}\int |\partial A|^2\,dx\Bigr)\\ -\int \mathsf{Weyl}_1(H_{A,V}+\eta,x)\,dx\Bigr),\tag{27.3.72}$$

(iii) And also with

$$\inf_{A}\Bigl(\int \Bigl(e_1(H_{A,V};x,x,0)-\mathsf{Weyl}_1(H_{A,V},x)\Bigr)\,dx+\\ \frac{1}{\kappa h^2}\int |\partial A|^2\,dx\Bigr).\tag{27.3.73}$$

(iv) We also can replace in Statement (i) $\mathsf{Tr}\bigl((\phi_r H_{A,V}\phi_r)^-\bigr)$ *by* $\mathsf{Tr}\bigl(\phi_r H^-_{A,V}\phi_r\bigr)$*. Here* $\phi\in\mathscr{C}_0^\infty(B(0,1))$*,* $\phi=1$ *in* $B(0,\frac{1}{2})$*,* $\phi_r=\phi(x/r)$*.*

Proof. Observe first that due to scaling $x\mapsto Zh^{-2}x$, $A\mapsto Z^{-1}hA$ and $\partial A\mapsto z^{-2}h^3\partial A$ one needs to consider only $Z=h=1$; all expressions on the left scale exactly as $Z^2h^{-2}S(Z\kappa)$.

(i) Let us compare

$$Q(r,\kappa,A):=\mathsf{Tr}\bigl((\phi_r H_{A,V}\phi_r)^-\bigr)-\int \mathsf{Weyl}_1(H_{A,V},x)\phi_r^2(x)\,dx+\frac{1}{\kappa}\int |\partial A|^2\,dx$$

and $Q(r',\kappa,A)$ with $r\ge 1$ and $r'\ge 2r$. Note that

$$Q(r',\kappa,A)\ge Q(r,(1+\epsilon)\kappa,A)+\\ \sum_{1\le j\le J}\Bigl(\mathsf{Tr}\bigl((\psi_{2^jr}H_{A,V}\psi_{2^jr})^-\bigr)-\int \mathsf{Weyl}_1(H_{A,V},x)\psi^2_{2^jr}(x)\,dx+\\ \frac{\epsilon}{2\kappa}\int |\partial A|^2\bar{\psi}^2_{2^jr}(x)\,dx\Bigr),$$

where ψ and $\bar{\psi}$ are smooth compactly supported functions, equal 0 in $B(0,\frac{1}{2})$ and $\bar{\psi}=1$ in the vicinity of $\mathsf{supp}(\psi)$, $J=\lfloor \log_2 r'/r\rfloor$, $\epsilon>0$ is arbitrarily small.

Therefore we can replace in the sum A by A_j and $\bar{\psi}_{2^jr}$ by 1 in $\int |\partial A|^2\bar{\psi}^2_{2^jr}(x)\,dx$; but then in the virtue of Section 27.2 each term in the sum is bounded from below by $-C'(\epsilon)\int \rho^3\ell^{-1}\bar{\psi}_t\,dx=-C'(\epsilon)t^{-\frac{1}{2}}$ with $t=2^jr$. Then

$$Q(r', \kappa, A) \ge Q(r, (1+\epsilon)\kappa, A) - C'(\epsilon)r^{-\frac{1}{2}}. \tag{27.3.74}$$

We know that $Q(r, (1+\epsilon)\kappa, A)$ is bounded from below by $-C(r)$ but now we conclude that this bound is uniform with respect to r, which implies that $2S(\kappa) := \liminf_{r\to+\infty} \inf_A Q(r, \kappa, A) > -\infty$. Further, (27.3.74) implies that

$$2S(\kappa) + C'(\epsilon)r^{-\frac{1}{2}} \ge \inf_A Q(r, (1+\epsilon)\kappa, A)$$

and therefore

$$\limsup_{r\to+\infty} \inf_A Q(r, \kappa, A) \le 2S((1+\epsilon)^{-1}\kappa). \tag{27.3.75}$$

Furthermore, plugging $A = 0$ we can see easily that $Q(r, \kappa, A)$ is uniformly bounded from above and therefore $2S(\kappa) < +\infty$; also our arguments imply that $\int |\partial A|^2\, dx$ is uniformly bounded for near optimizers and therefore $S(\kappa)$ is continuous with respect to $\kappa < \kappa^*$; combining with (27.3.75) we arrive to Statement (i).

(ii) Similarly, (27.3.74) holds with $H_{A,V}$ replaced by $H_{A,V} + \eta$ and then we can take $r' = \infty$ and apply $\inf_A$ to both sides arriving to

$$\begin{aligned}\inf_A \Bigl(\operatorname{Tr}\bigl((H_{A,V}+\eta)^-\bigr) - \int \mathsf{Weyl}_1(H_{A,V+\eta}, x)\, dx + \frac{1}{\kappa}\int |\partial A|^2\, dx \Bigr) \ge \\ \inf_A \Bigl(\operatorname{Tr}\bigl((\phi_r(H_{A,V}+\eta)\phi_r)^-\bigr) - \int \mathsf{Weyl}_1(H_{A,V+\eta}, x)\phi_r^2(x)\, dx + \\ \frac{1}{(1+\epsilon)\kappa}\int |\partial A|^2 \Bigr)\, dx - C'(\epsilon)r^{-\frac{1}{2}}.\end{aligned}$$

After this as $\eta \to +0$ the right-hand expression tends to itself with $\eta = 0$; tending $r \to +\infty$ we get there $2S((1+\epsilon)\kappa)$ in virtue of Statement (i) and tending $\epsilon \to +0$ we arrive to

$$\begin{aligned}\liminf_{\eta\to+0} \inf_A \Bigl(\operatorname{Tr}\bigl((H_{A,V}+\eta)^- V - \int \mathsf{Weyl}_1(H_{A,V+\eta}, x)\, dx + \\ \frac{1}{\kappa}\int |\partial A|^2\, dx \Bigr) \ge 2S(\kappa).\end{aligned} \tag{27.3.76}$$

On the other hand, consider

$$\operatorname{Tr}\bigl((H_{A,V}+\eta)^-\bigr) - \int \mathsf{Weyl}_1(H_{A,V+\eta}, x)\, dx + \frac{1}{\kappa}\int |\partial A|^2\, dx$$

and replace $\mathsf{Tr}\bigl((H_{A,V}+\eta)^-\bigr)$ by

$$\underbrace{\mathsf{Tr}\bigl((H_{A,V}+\eta)^-\phi_r^2\bigr)+\frac{1}{\kappa}\int|\partial A|^2\,dx}+\mathsf{Tr}\bigl((H_{A,V}+\eta)^-(1-\phi_r^2)\bigr). \tag{27.3.77}$$

Let A be a minimizer of the first expression; then in virtue of Propositions 27.2.24–27.2.26 this minimizer is sufficiently "good" on ϵr-vicinity of $\mathsf{supp}(1-\phi_r^2)$ and also the the difference between the second term and its Weyl expression does not exceed $Cr^{-\frac{1}{2}}$; one can prove it easily by $\ell(x)$-admissible partition of unity as in Part (i) of the proof and we leave details to the reader.

Observe that the first term in (27.3.77) is $\inf_A \mathsf{Tr}\bigl(\phi_r(H_{A,V}+\eta)^-\phi_r\bigr)$. In this expression we can take limit as $\eta\to+0$ just setting $\eta=0$ and therefore the left-hand expression in (27.3.76) with $\liminf$ replaced by $\limsup$ does not exceed

$$\inf_A\Bigl(\mathsf{Tr}(\phi_r H^-_{A,V}\phi_r)-\int \mathsf{Weyl}_1(H_{A,V},x)\phi_r^2(x)\,dx+\frac{1}{\kappa}\int|\partial A|^2\,dx\Bigr)+Cr^{-\frac{1}{2}};$$

taking limit as $r\to+\infty$ we conclude that the left-hand expression in (27.3.76) with $\liminf$ replaced by $\limsup$ does not exceed

$$\liminf_{r\to+\infty}\inf_A\Bigl(\mathsf{Tr}(\phi_r H^-_{A,V}\phi_r)-\int \mathsf{Weyl}_1(H_{A,V},x)\phi_r^2(x)\,dx+\frac{1}{\kappa}\int|\partial A|^2\,dx\Bigr).$$

This expression does not exceed (27.3.71) and therefore combining with (27.3.76) we prove Statements (ii) and (iv).

(iii) Similarly,

$$\int\Bigl(e_1(H_{A,V};x,x,0)-\mathsf{Weyl}_1(H_{A,V},x)\Bigr)\phi_r^2(x)\,dx+\frac{1}{\kappa}\int|\partial A|^2\,dx\ge \\ \inf_A\Bigl(\mathsf{Tr}\bigl((\phi_r H_{A,V}\phi_r)^-\bigr)-\int \mathsf{Weyl}_1(x)\phi_r^2(x)\,dx+\frac{1}{\kappa}\int|\partial A|^2\Bigr)-Cr^{-\frac{1}{2}}$$

and therefore

$$\inf_A\liminf_{r\to\infty}\int\Bigl(e_1(H_{A,V};x,x,0)-\mathsf{Weyl}_1(H_{A,V},x)\Bigr)\phi_r^2(x)\,dx+ \\ \frac{1}{\kappa}\int|\partial A|^2\,dx\ge 2S(\kappa).$$

On the other hand, as in Part (ii) of the proof, taking A to be a minimizer of the first expression in (27.3.77), we see that

$$\inf_A \limsup_{r\to\infty} \int \Bigl(e_1(H_{A,V};x,x,0) - \mathsf{Weyl}_1(H_{A,V},x)\Bigr)\phi_r^2(x)\,dx + \frac{1}{\kappa}\int |\partial A|^2\,dx \le 2S(\kappa)$$

and Statement (iii) has been proven. □

Remark 27.3.19. (i) Statements similar to (i), (ii) were proven in L. Erdös, S. Fournais, and J. P. Solovej [3] (see Theorem 2.4 and Lemma 2.5 respectively).

(ii) Again as observed in in L. Erdös, S. Fournais, and J. P. Solovej [3] we do not know if

(a) $S(\kappa) < S(0)$ for $\kappa > 0$ or just

(b) $S(\kappa) = S(0)$ for $\kappa < \kappa^*$ and $S(\kappa) = -\infty$ for $\kappa > \kappa^*$.

If we knew that the optimizer is unique, then obviously $A = 0$ and it would be relatively easy but rather unexciting the latter case.

(iii) While we assumed that $\kappa < \kappa^*$ with $\kappa^* > 0$ and it is possible that $S(\kappa) = -\infty$ as $\kappa > \kappa^*$ with some $\kappa^* < \infty$ we are not aware about any proof of this, so in fact it could happen that $\kappa^* = +\infty$ and then condition $\kappa < \kappa^*$ is superficial and one needs to study asymptotics of $S(\kappa)$ as $\kappa \to +\infty$.

Proposition 27.3.20. *For* $0 < \kappa < \kappa'$

$$S(\kappa') \le S(\kappa) \le S(\kappa') + C\kappa'(\kappa^{-1} - \kappa'^{-1}). \tag{27.3.78}$$

Proof. Monotonicity of $S(\kappa)$ is obvious.

Let $0 < \kappa < \kappa' < \kappa'' \le \kappa^*$. Then for any $\varepsilon > 0$ if $r = r_\varepsilon$ is large enough then the left-hand expression in (27.3.71) for κ' (without $\inf$ and $\lim$) is greater than $S(\kappa'') - \varepsilon + (\kappa'^{-1} - \kappa''^{-1})\|\partial A\|^2$; also, if A is an almost minimizer there, it is less than $S(\kappa') + \varepsilon$.

Therefore $(\kappa'^{-1} - \kappa''^{-1})\|\partial A\|^2 \le |S(\kappa'') - S(\kappa')| + 2\varepsilon$. But then

$$S(\kappa) - \varepsilon \le S(\kappa') + \varepsilon + (\kappa^{-1} - \kappa'^{-1})\|\partial A\|^2 \le S(\kappa') + \varepsilon + C(\kappa^{-1} - \kappa'^{-1})(\kappa'^{-1} - \kappa''^{-1})^{-1}\bigl(|S(\kappa'') - S(\kappa')| + 2\varepsilon\bigr)$$

and therefore

$$(\kappa^{-1} - \kappa'^{-1})^{-1}|S(\kappa) - S(\kappa')| \le (\kappa'^{-1} - \kappa''^{-1})^{-1}|S(\kappa') - S(\kappa'')| \tag{27.3.79}$$

which for $\kappa'' = \kappa^*$ implies (27.3.78). □

Remark 27.3.21. Using global equation (27.2.14) we conclude that for $Z = h = 1$

$$|\partial^\alpha A| \le C\kappa \ell^{-1-|\alpha|} \qquad \text{if } \ell \ge 1,\ |\alpha| \le 1, \tag{27.3.80}$$

$$|\partial^\alpha A| \le C\kappa \qquad \text{if } \ell \le 1,\ |\alpha| \le 1, \tag{27.3.81}$$

$$\|\partial A\|^2 \le C\kappa^2. \tag{27.3.82}$$

Then

$$S'(\kappa) \le C, \qquad |S(\kappa(1+\eta)) - S(\eta)| \le C\kappa\eta. \tag{27.3.83}$$

Main Theorem

In the "atomic" case $M = 1$ we arrive instantly to the following theorem:

Theorem 27.3.22. *Let $M = 1$ and $\kappa \le \kappa^*$. Then*

(i) Asymptotics holds

$$\mathsf{E}^* = \int \mathsf{Weyl}_1(x)\, dx + 2z^2 S(z\kappa)h^{-2} + O(h^{-\frac{4}{3}}\kappa|\log\kappa|^{\frac{1}{3}} + h^{-1}). \tag{27.3.84}$$

(ii) If $\kappa = o(h^{\frac{1}{3}}|\log h|^{-\frac{1}{3}})$, then

$$\mathsf{E}^* = \int \mathsf{Weyl}_1^*(x)\, dx + 2z^2 S(z\kappa)h^{-2} + o(h^{-1}). \tag{27.3.85}$$

Proof. If A satisfies the minimizer properties, then in virtue of Proposition 27.3.16

$$\begin{aligned}\mathsf{Tr}^-(H_{A,V}) - \int \mathsf{Weyl}_1(x)\, dx \equiv \mathsf{Tr}^-(H_{A,V^0}) - \int \mathsf{Weyl}_1^0(x)\, dx \\ + O(h^{-\frac{4}{3}}\kappa|\log\kappa|^{\frac{1}{3}} + h^{-1})\end{aligned} \tag{27.3.86}$$

and adding magnetic energy and plugging either minimizer for V or for V^0 we get

$$\inf_A\Bigl(\operatorname{Tr}^-(H_{A,V}) - \int \mathsf{Weyl}_1(x)\,dx + \frac{1}{\kappa h^2}\int |\partial A|^2\,dx\Bigr) \lesseqgtr \inf_A\Bigl(\operatorname{Tr}^-(H_{A,V^0}) - \int \mathsf{Weyl}_1^0(x)\,dx + \frac{1}{\kappa h^2}\int |\partial A|^2\,dx\Bigr) \pm C(h^{-\frac{4}{3}}\kappa|\log\kappa|^{\frac{1}{3}} + h^{-1}). \tag{27.3.87}$$

Obviously if V (and surely V^0) are not sufficiently fast decaying at the infinity, the left (and for sure the right hand) expression in (27.3.86) should be regularized as in Subsubsection *27.3.5.1. Coulomb Potential.* However for potential decaying fast enough (faster than $|x|^{-2-\delta}$) the regularization is not needed.

For V^0 we have an exact expression which concludes the proof of Statement (i).

The proof of Statement (ii) is similar albeit with the small improvement, based on the behavior of the classical dynamics (without magnetic field) exactly as in Chapter 25. □

27.3.6 Several Singularities

Consider now the "molecular" case $M \ge 2$. Then we need more delicate arguments.

Decoupling of Singularities

Consider partition of unity $1 = \sum_{0\le m\le M}\psi_m^2$ where ψ_m is supported in $\frac{1}{3}a$-vicinity of y_m for $m = 1, \dots, M$ and $\psi_0 = 0$ in $\frac{1}{4}a$-vicinities of y_m ("near-nuclei" and "between-nuclei" partition elements).

Estimate from above. Then

$$\operatorname{Tr}(H_{A,V}^-) = \sum_{0\le m\le M}\operatorname{Tr}(\psi_m H_{A,V}^-\psi_m), \tag{27.3.88}$$

and to estimate E^* from the above we impose an extra condition to A:

$$A = 0 \qquad \text{for}\ \ \ell(x) \ge \frac{1}{5}a. \tag{27.3.89}$$

Then in this framework we estimate

$$\operatorname{Tr}^-(\psi_0 H^-_{A,V}\psi_0) - \int \mathsf{Weyl}_1(x)\psi_0^2(x)\,dx \le Ch^{-1}a^{-\frac{1}{2}}. \tag{27.3.90}$$

Proof of this inequality is trivial by using ℓ-admissible partition and applying results of the theory without any magnetic field.

Thus, to estimate E^* from above[17)] we just need to estimate from above the minimum with respect to A satisfying (27.3.89) of the expression

$$\operatorname{Tr}(\psi_m H^-_{A,V}\psi_m) - \int \mathsf{Weyl}_1(x)\psi_m^2(x)\,dx + \frac{1}{\kappa h^2}\int_{\{\ell_m(x)\le \frac{1}{5}a\}} |\partial A|^2\,dx. \tag{27.3.91}$$

Estimate from below. In this case we use the same partition of unity $\{\psi_m^2\}_{j=0,1,\dots,M}$ and estimate

$$\operatorname{Tr}(H^-_{A,V}) \ge \sum_{0\le m\le M} \operatorname{Tr}^-(\psi_m H_{A,V'}\psi_m) \tag{27.3.92}$$

with

$$V' = V + 2h^2 \sum_{0\le m\le M} (\partial\psi)^2, \tag{27.3.93}$$

and we also use decomposition

$$\int |\partial A|^2\,dx = \sum_{0\le m\le M}\int \omega_m^2 |\partial A|^2\,dx \tag{27.3.94}$$

with

$$\omega_m(x) = 1 \ \text{ if }\ \ell_m(x)\le \frac{1}{10}a,\quad \omega_m(x)\ge 1 - C\varsigma \ \text{ if }\ \ell_m(x)\le \frac{1}{2}a \qquad \text{for}\ \ m=1,\dots,M, \tag{27.3.95}$$

$$\omega_0 \ge \epsilon_0\varsigma \quad \text{if}\ \ \ell(x)\ge \frac{1}{5}a. \tag{27.3.96}$$

So far $\varsigma > 0$ is a constant but later it will become a small parameter. Then since

$$\operatorname{Tr}^-(\psi_0 H_{A,V'}\psi_0) - \int \mathsf{Weyl}_1(x)\psi_0^2(x)\,dx + \frac{1}{\kappa h^2}\int \omega_0^2|\partial A|^2\,dx \ge Ch^{-1}a^{-\frac{1}{2}} \tag{27.3.97}$$

(again proven by partition) in virtue of the previous Section 27.2 we are left with the estimates from below for

---

17) Modulo error in (27.3.51).

$$\mathsf{Tr}^{-}(\psi_m H_{A,V'}\psi_m) - \int \mathsf{Weyl}_1(x)\psi_m^2(x)\,dx + \frac{1}{\kappa h^2}\int \omega_m^2|\partial A|^2\,dx. \tag{27.3.98}$$

Remark 27.3.23. (i) Note that the error in Weyl_1 when we replace V' there by V does not exceed $Ch^{-1}(1+a^{-\frac{1}{2}})$ which is less than the error in (27.3.51). Here we can also assume that A satisfies (27.3.89); we need just to replace ς by $\epsilon_0\varsigma$ in (27.3.95)–(27.3.96).

(ii) We can further go down by replacing $\mathsf{Tr}^{-}(\psi_m H_{A,V'}\psi_m)$ by $\mathsf{Tr}(\psi_m H^{-}_{A,V'}\psi_m)$.

(iii) Therefore we basically have the same object for both estimates albeit with marginally different potentials (V in the estimate from above and V' in the estimate from below) and with a weight ω_m^2 satisfying (27.3.95)–(27.3.96); in both cases $\omega=1$ if $\ell(x)\le \frac{1}{10}a$ but in the estimate from above $\omega(x)$ grows to C_0 and in the estimate from below $\omega(x)$ decays to ς if $\ell(x)\ge\frac{1}{3}a$ and in both cases condition (27.3.89) could be either imposed or skipped.

(iv) From now on we consider a single singularity at 0 and we skip subscript m. However if there was a single singularity from the beginning, all arguments of this and forthcoming paragraphs would be unnecessary.

Scaling. Now we apply scaling arguments:

(i) We are done as $Z\asymp 1$ but as $Z\ll 1$[18] we need a bit more fixing. The problem is that $V\asymp Z\ell^{-1}$ only for $|x|\le aZ$; otherwise $V\lesssim a^{-1}$ (where we still assume that $a\le 1$). To deal with this we apply in the zone $\{x\colon aZ\le |x|\le a\}$ the same procedure as before and its contribution to the error will be $Ch^{-1}a^{-\frac{1}{2}}$ as $\rho=a^{-\frac{1}{2}}$ here. Actually we also need to keep $|x|\ge Z^{-1}h^2$; so we assume that $Z^{-1}h^2\le Za$, i.e. $Z\ge a^{-\frac{1}{2}}h$.

Now let us scale $x\mapsto x'=x(aZ)^{-1}$, and multiply $H_{a,V}$ by a and therefore also multiply A by $a^{\frac{1}{2}}$, so $A\mapsto A'=a^{\frac{1}{2}}A$, $h\mapsto h'=ha^{-\frac{1}{2}}Z^{-1}$; then the magnetic energy becomes

$$\kappa^{-1}h^{-2}Z\int \omega^2(x)|\partial' A'|^2\,dx',$$

where factors a^{-1} and aZ come from substitution $A=a^{-\frac{1}{2}}A'$ and scaling respectively. We need to multiply it by a (since we multiplied an operator); then plugging $h^{-2}=h'^{-2}a^{-1}Z^{-2}$ we get the same expression as before but with $Z'=1$, $a'=1$ and $h'=ha^{-\frac{1}{2}}Z^{-1}\le 1$ and $\kappa'=\kappa Z$ instead of h and κ.

[18] Since Z denotes Z_m now we assume only that $Z_1+\ldots+Z_M\asymp 1$.

If we prove here an error $O\bigl(h'^{-1}+\kappa'|\log\kappa'|^{\frac{1}{3}}h'^{-\frac{4}{3}}\bigr)$, then the final error will be this expression multiplied by a^{-1}, i.e. $O\bigl(a^{-\frac{1}{2}}Zh^{-1}+\kappa a^{-\frac{1}{2}}Z^{\frac{7}{3}}|\log\kappa Z|^{\frac{1}{3}}h^{-\frac{4}{3}}\bigr)$, which is less than the same expression with $Z=1$.

(ii) On the other hand, let $Z\le a^{-\frac{1}{2}}h$. Recall, we assume that $a\ge C_0h^2$. Then we can apply the same arguments as before but with $\bar{Z}=a^{-\frac{1}{2}}h$ and we arrive to the same situation as before albeit with $h'=1$, $a'=1$, $\kappa'=\kappa a^{-\frac{1}{2}}h$ and with $Z'=Z\bar{Z}^{-1}$. Then we have the trivial error estimate $O(a^{-1})$ which is less than $O(a^{-\frac{1}{2}}h^{-1})$.

Main Results

Combining results of the previous subsubsections and paragraphs with Proposition 27.3.9 we arrive to

Theorem 27.3.24. *Let $M\ge 2$, $\kappa\le\kappa^*$ and (27.3.38) hold with $\nu>\frac{4}{3}$. Then*

(i) The following asymptotics holds

$$\mathsf{E}^* = \int \mathsf{Weyl}_1(x)\,dx + 2\sum_{1\le m\le M} z_m^2 S(z_m\kappa)h^{-2} + O(R_1+R_2) \tag{27.3.99}$$

with

$$R_1 = \begin{cases} h^{-1}+\kappa|\log\kappa|^{\frac{1}{3}}h^{-\frac{4}{3}} & \text{if } a\ge 1,\\ a^{-\frac{1}{2}}h^{-1}+\kappa|\log\kappa|^{\frac{1}{3}}a^{-\frac{1}{3}}h^{-\frac{4}{3}} & \text{if } h^2\le a\le 1\end{cases} \tag{27.3.100}$$

and

$$R_2=\kappa h^{-2}\begin{cases} a^{-3} & \text{if } a\ge|\log h|^{\frac{1}{3}},\\ |\log h^2a^{-1}|^{-1} & \text{if } h^2\le a\le|\log h|^{\frac{1}{3}}.\end{cases} \tag{27.3.101}$$

(ii) If $\kappa=o(h^{\frac{1}{3}}|\log h|^{-\frac{1}{3}})$, $\kappa a^{-3}=o(h)$ and $a^{-1}=o(1)$, then

$$\mathsf{E}^* = \int \mathsf{Weyl}_1^*(x)\,dx + 2\sum_{1\le m\le M} z_m^2 S(z_m\kappa)h^{-2} + o(h^{-1}). \tag{27.3.102}$$

Proof. To prove theorem we need to prove the following estimate

$$\frac{1}{\kappa}\|\partial A\|^2_{\{b\le\ell(x)\le 2b\}},\le Cb^{-3} \tag{27.3.103}$$

where $r_* \le b \le a$ is a "cut-off". On the other hand, we know that

$$\frac{1}{\kappa}\|\partial A\|^2 = -\frac{\partial S}{\partial \kappa} = O(1) \tag{27.3.104}$$

and we need to recover the last factor in the definition of R_2.

For $a \ge 1$ we can have κa^{-3} because in virtue of (27.3.41) the square of the partial norm in (27.3.104) does not exceed $Ca^{-3}\kappa^2$.

On the other hand, for $h^2 \le r_* \le a$ we can select $b : r_* \le b \le a$ such that the partial norm in (27.3.104) does not exceed $C|\log(a/h^2)|^{-1} \cdot \|\partial A\|^2$. □

Remark 27.3.25. (i) For $a \le |\log h|$ we do not need assumption (27.3.38).

(ii) Following arguments of Section 12.6 estimates (27.3.85) and (27.3.104) could be improved to $O(h^{-1+\delta})$ provided $a \ge h^{-\delta_1}$, $\kappa \le h^{\frac{1}{3}+\delta_1}|\log h|^{-\frac{1}{3}}$ and $\kappa \le a^3 h^{1+\delta_1}$.

Problems and Remarks

The following problem seems to be really challenging and we have no idea how to approach it:

Problem 27.3.26. (i) For $\kappa \in [0, \kappa^*]$ with small enough $\kappa^* > 0$ does $S(\kappa)$ really depend on κ or $S(\kappa) = S(0)$ (see Remark 27.3.19)?

(ii) If $S(\kappa)$ really depends on κ, what is asymptotic behavior of $S(\kappa) - S(0)$ as $\kappa \to +0$: can one improve $S(\kappa) - S(0) = O(\kappa)$?

(iii) Do we really need an assumption $\kappa \in [0, \kappa^*]$ (again see Remark 27.3.19)?

(iv) Can one improve estimates to minimizer?

27.4 Asymptotics of the Ground State Energy

27.4.1 Problem

Now we are ready to tackle our original object (27.1.2)–(27.1.3). So, let us consider our usual quantum Hamiltonian

$$\mathsf{H} = \sum_{1 \le j \le N} H^0_{x_j} + \sum_{1 \le j < k \le N} |x_j - x_k|^{-1} \tag{27.4.1}$$

in

$$\mathfrak{H} = \bigwedge_{1\le n\le N} \mathsf{H}, \qquad \mathsf{H} = \mathscr{L}^2(\mathbb{R}^3, \mathbb{C}^2) \tag{27.4.2}$$

with

$$H^0 = \bigl((i\nabla - A)\cdot \boldsymbol{\sigma}\bigr)^2 - V(x). \tag{27.4.3}$$

We are interested in the *ground state energy* $\mathsf{E}^*_N(A)$ of our system i.e. in the lowest eigenvalue of the operator H on $\mathfrak{H}$:

$$\mathsf{E}^*_N(0) = \inf \operatorname{Spec}(\mathsf{H}) \qquad \text{on } \ \mathfrak{H} \tag{27.4.4}$$

if $A = 0$ and more generally in

$$\mathsf{E}^*_N = \inf_A \Bigl(\inf \operatorname{Spec}_{\mathfrak{H}}(\mathsf{H}) + \frac{1}{\alpha}\int |\nabla\times A|^2\,dx\Bigr), \tag{27.4.5}$$

where

$$V(x) = \sum_{1\le m\le M} \frac{Z_m}{|x-\mathsf{y}_m|} \tag{27.4.6}$$

$$N \asymp Z \gg 1, \qquad Z := Z_1 + \ldots + Z_M, \qquad Z_1 > 0, \ldots, Z_M > 0, \tag{27.4.7}$$

M is fixed, under assumption

$$0 < \alpha \le \kappa^* Z^{-1} \tag{27.4.8}$$

with sufficiently small constant $\kappa^* > 0$.

Our purpose is to derive an asymptotics

$$\mathsf{E}^*_N \approx \mathcal{E}^{\mathsf{TF}}_N + \sum_{1\le m\le M} 2Z_m^2 S(\alpha Z_m) \tag{27.4.9}$$

and estimate an error (usually) provided

$$b := \min_{1\le m<m'\le M} |\mathsf{y}_m - \mathsf{y}_{m'}| \ge Z^{-\frac{1}{3}}. \tag{27.4.10}$$

Recall that the Thomas-Fermi potential W^{TF} and the Thomas-Fermi density ρ^{TF} satisfy equations

$$\rho^{\mathsf{TF}} = \frac{1}{3\pi^2}(W^{\mathsf{TF}} + \nu)_+^{\frac{3}{2}} \tag{27.4.11}$$

and

$$W^{\mathsf{TF}} = V^0 + |x|^{-1} * \rho^{\mathsf{TF}}, \tag{27.4.12}$$

where ν is a chemical potential.

27.4.2 Lower Estimate

Consider corresponding to H quadratic form exactly as in Sections 25.2 and 26.6

$$\begin{multline}\langle \mathsf{H}\Psi,\Psi\rangle = \sum_j (H^0_{x_j}\Psi,\Psi) + \bigl(\sum_{1\le j<k\le N} |x_j-x_k|^{-1}\Psi,\Psi\bigr) =\\ \sum_j (H_{x_j}\Psi,\Psi) + ((V-W)\Psi,\Psi) + \bigl(\sum_{1\le j<k\le N} |x_j-x_k|^{-1}\Psi,\Psi\bigr)\end{multline}\tag{27.4.13}$$

with

$$H = \bigl((i\nabla - A)\cdot \boldsymbol{\sigma}\bigr)^2 - W(x)\tag{27.4.14}$$

where we select W later. By Lieb-Oxford inequality the last term is estimated from below:

$$\langle \sum_{1\le j<k\le N} |x_j-x_k|^{-1}\Psi,\Psi\rangle \ge \frac{1}{2}\mathsf{D}(\rho_\Psi,\rho_\Psi) - C\int \rho_\Psi^{\frac{4}{3}}\,dx,\tag{27.4.15}$$

where

$$\rho_\Psi(x) = N\int |\Psi(x,x_2,\ldots,x_N)|^2\,dx_2\cdots dx_N\tag{27.4.16}$$

is a spatial density associated with Ψ and

$$\mathsf{D}(\rho,\rho') := \iint |x-y|^{-1}\rho(x)\rho'(y)\,dxdy.\tag{27.4.17}$$

Therefore again repeating arguments of Section 25.2 we estimate H from below:

$$\begin{multline}\langle \mathsf{H}\Psi,\Psi\rangle \ge\\ \sum_j (H_{x_j}\Psi,\Psi) - 2((V-W)\Psi,\Psi) + \frac{1}{2}\mathsf{D}(\rho_\Psi,\rho_\Psi) - C\int \rho_\Psi^{\frac{4}{3}}\,dx =\\ \sum_j (H_{x_j}\Psi,\Psi) - \mathsf{D}(\rho,\rho_\Psi) + \frac{1}{2}\mathsf{D}(\rho_\Psi,\rho_\Psi) - C\int \rho_\Psi^{\frac{4}{3}}\,dx =\\ \sum_j (H_{x_j}\Psi,\Psi) - \frac{1}{2}\mathsf{D}(\rho,\rho) + \frac{1}{2}\mathsf{D}(\rho-\rho_\Psi,\rho-\rho_\Psi) - C\int \rho_\Psi^{\frac{4}{3}}\,dx\end{multline}\tag{27.4.18}$$

swhere

$$W - V = |x|^{-1} * \rho. \tag{27.4.19}$$

Note that due to antisymmetricity of Ψ

$$\sum_j (H_{x_j}\Psi, \Psi) \ge \sum_{1\le j\le N:\, \lambda_j<0} \lambda_j \ge \operatorname{Tr}^-(H), \tag{27.4.20}$$

where λ_j are eigenvalues of H.

To estimate the last term in (27.4.18) we reproduce the proof of Lemma 4.3 from L. Erdös, S. Fournais and J. P. Solovej [3]:

According to magnetic Lieb–Thirring inequality for $U \ge 0$:

$$\sum_{j\le N} \langle (H^0_{x_j} - U)\Psi, \Psi\rangle \ge -C\int U^{5/2}\,dx - C\gamma^{-3}U^4\,dx - \gamma\int B^2\,dx \tag{27.4.21}$$

where $B = \nabla\times A$, $\gamma > 0$ is arbitrary. Then, selecting $U = \beta\min(\rho_\Psi^{5/3}, \gamma\rho_\Psi^{4/3})$ with $\beta > 0$ sufficiently small but independent from γ, we ensure that $\frac{1}{2}U\rho_\Psi \ge CU^{5/2} + C\gamma^{-3}U^4$ and then

$$\sum_{j\le N} \langle (H^0_{x_j})\Psi, \Psi\rangle \ge \epsilon\int \min(\rho_\Psi^{5/3}, \gamma\rho^{4/3})\,dx, -\gamma\int B^2\,dx, \tag{27.4.22}$$

which implies

$$\begin{aligned}\int \rho_\Psi^{4/3}dx \le \gamma^{-1}\int \min(\rho_\Psi^{5/3}, \gamma\rho^{4/3})\,dx + \gamma\int \rho_\Psi\,dx \le \\ c\gamma^{-1}\sum_{j:\lambda_j<0} \langle (H^0_{x_j})\Psi, \Psi\rangle + c\int B^2\,dx + c\gamma N\end{aligned} \tag{27.4.23}$$

where we use $\int \rho_\Psi\,dx = N$.

Remark 27.4.1. As one can prove easily (see also L. Erdös, S. Fournais and J. P. Solovej [3]) that

$$\sum_{j\le N} \langle (H^0_{x_j})\Psi, \Psi\rangle \le CZ^{\frac{4}{3}}N \tag{27.4.24}$$

even if $N \not\asymp Z$; then we conclude that

$$\int \rho_\Psi^{4/3}\,dx \le CZ^{\frac{2}{3}}N + C_1\int B^2\,dx. \tag{27.4.25}$$

It is sufficient unless we want to recover Dirac-Schwinger terms which unfortunately is possible only if $\alpha \ll Z^{-\frac{10}{9}}|\log Z|^{-\frac{1}{3}}$. To recover remainder estimate $o(Z^{\frac{5}{3}})$ (or marginally better) we just apply Theorem 26.A.2. We will do it later (see Theorem 27.4.5).

Therefore skipping the non-negative third term in the right-hand expression of (27.4.18) we conclude that

$$\begin{aligned} \langle \mathsf{H}\Psi,\Psi\rangle + \frac{1}{\alpha}\int |\nabla\times A|^2\,dx \ge \\ \operatorname{Tr}^-(H) + (\frac{1}{\alpha} - C_1)\int |\nabla\times A|^2\,dx - \frac{1}{2}\mathsf{D}(\rho,\rho) - CZ^{\frac{5}{3}}. \end{aligned} \tag{27.4.26}$$

Applying Theorem 27.3.24 we conclude that

(27.4.27) The sum of the first and the second terms in the right-hand expression of (27.4.26) is greater than

$$\mathcal{E}^{\mathsf{TF}} + \sum_m 2Z_m^2 S(\alpha Z_m) - CZ^{\frac{4}{3}}(R_1 + R_2)$$

with R_1 and R_2 defined by (27.3.100) and (27.3.101) respectively with $\kappa = \alpha Z$, $h = Z^{-\frac{1}{3}}$ and

$$a := Z^{\frac{1}{3}} \min_{1\le m<m'\le M} |\mathsf{y}_m - \mathsf{y}_{m'}|. \tag{27.4.28}$$

To prove this claim one needs just to rescale

$$\begin{aligned} x\mapsto xZ^{\frac{1}{3}},\quad a\mapsto aZ^{\frac{1}{3}},\quad W\mapsto Z^{-\frac{4}{3}}W, \\ A\mapsto A,\quad \nabla\times A\mapsto Z^{\frac{1}{3}}\nabla\times A \end{aligned} \tag*{(27.4.29)$_{1-5}$}$$

and introduce

$$h = Z^{-\frac{1}{3}},\quad \kappa = \alpha Z. \tag{27.4.30}$$

Observe that due to $(27.4.29)_3$ we need to multiply our estimate by $Z^{\frac{4}{3}}$.

Here one definitely needs the regularity properties like in Section 27.3 but we have them since $\rho = \rho^{\mathsf{TF}}$, $W = W^{\mathsf{TF}}$. Also one can see easily that "$-C_1$" brings correction not exceeding $C_2\alpha Z^2$ as $\alpha Z \le 1$.

Meanwhile for $\rho = \rho^{\mathsf{TF}}$, $W = W^{\mathsf{TF}}$

$$\frac{2}{15\pi^2}\int W^{\frac{5}{2}}\,dx - \frac{1}{2}\mathsf{D}(\rho,\rho) = \mathcal{E}^{\mathsf{TF}}. \tag{27.4.31}$$

Lower estimate of Theorem 27.4.3 below has been proven.

Remark 27.4.2. $\rho = \rho^{\mathsf{TF}}$, $W = W^{\mathsf{TF}}$ delivers the maximum of the right-hand expression of (27.4.31) among ρ, W satisfying (27.4.19).

27.4.3 Upper Estimate

Upper estimate is easy. Plugging as in Section 25.2 Ψ, the *Slater determinant* (25.2.16) of $\psi_1,\dots,\psi_N$, where $\psi_1,\dots,\psi_N$ are eigenfunctions of $H_{A,W}$ we get

$$\begin{aligned}\langle \mathsf{H}\Psi,\Psi\rangle = \mathsf{Tr}^-(H_{A,W}-\lambda_N) + \lambda_N N +\\ \int (W-V)(x)\rho_\Psi(x)\,dx + \frac{1}{2}\mathsf{D}(\rho_\Psi,\rho_\Psi) -\\ \frac{1}{2}N(N-1)\iint |x_1-x_2|^{-1}|\Psi(x_1,x_2,x_3,\dots,x_N|^2\,dx_1\cdots dx_N,\end{aligned} \tag{27.4.32}$$

where we do not care about the last term since we drop it (again as long as we cannot get sharp enough estimate) and the first term in the second line is in fact $-\mathsf{D}(\rho,\rho_\Psi)$, provided (27.4.19) holds. Thus we get

$$\begin{aligned}\mathsf{Tr}^-(H_{A,W}-\lambda_N) + \lambda_N N - \frac{1}{2}\mathsf{D}(\rho,\rho) + \frac{1}{2}\mathsf{D}(\rho_\Psi-\rho,\rho_\Psi-\rho) +\\ \frac{1}{\alpha}\int |\partial A|^2\,dx,\end{aligned} \tag{27.4.33}$$

where we added the magnetic energy. Definitely we have several problems here: λ_N depends on A and there may be less than N negative eigenvalues.

However in the latter case we can obviously replace N by the lesser number $N' := \max(n\le N, \lambda_n\le 0)$ since E^*_N is decreasing function of N. In this case the first term in (27.4.33) would be just $\mathsf{Tr}^-(H_{A,W})$ and the second would be 0. Then we apply theory of the previous Section 27.3 immediately without extra complications.

Consider A a minimizer (or its mollification) for operator $H_{A,W}-\mu$ with potential $W=W^{\mathsf{TF}}$ and $\mu\le 0$. Then

$$\mathsf{N}(\mu)\coloneqq \#\{\lambda_k<\mu\}=\int (W+\mu)_+^{\frac{3}{2}}\,dx+O(Z^{\frac{2}{3}}). \tag{27.4.34}$$

One can prove (27.4.34) easily using the regularity properties of A established in the previous Section 27.3 and the same rescaling (27.4.29)–(27.4.30) as before. We leave this easy proof to the reader.

Therefore, repeating arguments of Subsubsection *25.4.2.1. Estimating* $|\lambda_N-\nu|$, we conclude that either $N\ge Z-C_0Z^{\frac{2}{3}}$ and then $|\nu|\le C_1Z^{\frac{8}{9}}$ and we can take $\mu=0$ and $|\lambda_{N'}|\le C_1Z^{\frac{8}{9}}$ or $N\le Z-C_0Z^{\frac{2}{3}}$ and then we take $\mu=\nu$, $|\lambda_N|\asymp|\nu|\asymp (Z-N)_+^{\frac{4}{3}}$ and $|\lambda_N-\nu|\le C_1|\nu|^{\frac{1}{4}}Z^{\frac{2}{3}}$.

After this, following again to arguments of Subsection 25.4.2, we conclude that

(27.4.35) Expression (27.4.33) without term $\frac{1}{2}\mathsf{D}(\rho_\Psi-\rho,\rho_\Psi-\rho)$ does not exceed

$$\mathcal{E}^{\mathsf{TF}}+\sum_m 2Z_m^2S(\alpha Z_m)+CZ^{\frac{4}{3}}(R_1+R_2)$$

with R_1 and R_2 defined by (27.3.100) and (27.3.101) respectively with $\kappa=\alpha Z$, $h=Z^{-\frac{1}{3}}$ and a defined by (27.4.28).

Now we need to estimate properly $\mathsf{D}(\rho_\Psi-\rho,\rho_\Psi-\rho)$ which as in i.e. Subsubsection *25.4.2.2. Estimating* D*-Term* does not exceed the sum of

$$\mathsf{D}(e(x,x,\mu)-\mathsf{Weyl}(x,\mu),\ e(x,x,\mu)-\mathsf{Weyl}(x,\mu)), \tag{27.4.36}$$

$$\mathsf{D}(e(x,x,\lambda_N)-\mathsf{Weyl}(x,\lambda_N),\ e(x,x,\lambda_N)-\mathsf{Weyl}(x,\lambda_N)) \tag{27.4.37}$$

and

$$\mathsf{D}(\mathsf{Weyl}(x,\mu)-\mathsf{Weyl}(x,\lambda_N),\ \mathsf{Weyl}(x,\mu)-\mathsf{Weyl}(x,\lambda_N)). \tag{27.4.38}$$

Next, following arguments of Subsubsection *25.4.2.2. Estimating* D-*Term*, one can prove easily that due to regularity properties of A both semiclassical (27.4.36) and (27.4.37) terms do not exceed $CZ^{\frac{5}{3}}$ and due to estimates for $|\lambda_N-\mu|$ the last term does (27.4.38) not exceed $CZ^{\frac{5}{3}}$ as well.

This concludes the proof of the upper estimate in Theorem 27.4.3 below.

27.4.4 Main Theorems

Theorem 27.4.3. *(i) Under assumptions* (27.4.7) *and* (27.4.8) *the following asymptotics holds*

$$\mathsf{E}_N^* = \mathcal{E}_N^{\mathsf{TF}} + \sum_{1\le m\le M} 2Z_m^2 S(\alpha Z_m) + O\bigl(Z^{\frac{4}{3}}(R_1 + R_2)\bigr) \tag{27.4.39}$$

with R_1 and R_2 defined by (27.3.100) *and* (27.3.101) *respectively with $\kappa = \alpha Z$, $h = Z^{-\frac{1}{3}}$ and a defined by* (27.4.28)*, $a = \infty$ for $M = 1$.*

(ii) In particular, under assumption (27.4.10) *the following asymptotics holds*

$$\mathsf{E}_N^* = \mathcal{E}_N^{\mathsf{TF}} + \sum_{1\le m\le M} 2Z_m^2 S(\alpha Z_m) + O\bigl(\alpha|\log(\alpha Z)|^{\frac{1}{3}} Z^{\frac{25}{9}} + Z^{\frac{5}{3}} + \alpha b^{-3} Z^2\bigr). \tag{27.4.40}$$

Recall that $\mathcal{E}_N^{\mathsf{TF}}$ is a *Thomas-Fermi energy* and $S(\alpha Z_m)Z_m^2$ are magnetic *Scott correction terms*.

Theorem 27.4.4. *(i) Let assumptions* (27.4.7) *and* (27.4.8) *be fulfilled and let $\Psi = \Psi_{\boldsymbol{A}}$ be a ground state for a near optimizer $\boldsymbol{A}$ of the original multiparticle problem. Then*

$$\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}},\, \rho_\Psi - \rho^{\mathsf{TF}}) \le CZ^{\frac{5}{3}}. \tag{27.4.41}$$

(ii) Furthermore, as $b \ge Z^{-\frac{1}{3}}$

$$\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}},\, \rho_\Psi - \rho^{\mathsf{TF}}) \le CZ^{\frac{5}{3}}\bigl(Z^{-\delta} + (bZ^{\frac{1}{3}})^{-\delta} + (\alpha Z)^{\delta}\bigr). \tag{27.4.42}$$

Proof. (i) Note that all the terms in estimates from below and from above are $O(Z^{\frac{5}{3}})$ except the common term

$$\operatorname{Tr}^-(H_{A,W} + \mu) + \frac{1}{\alpha}\int |\nabla \times A|^2\, dx, \tag{27.4.43}$$

where A is a minimizer for this term and therefore estimate (27.4.41) has been proven because estimate from below also contains $\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}},\, \rho_\Psi - \rho^{\mathsf{TF}})$.

(ii) To prove Statement (ii) one needs

(a) To improve estimate (27.4.34) to

$$\mathsf{N}(\mu) = \int (W+\mu)_+^{\frac{3}{2}}\,dx + O\bigl(Z^{\frac{2}{3}}\bigl[Z^{-\delta} + (bZ^{\frac{1}{3}})^{-\delta} + (\alpha Z)^{\delta}\bigr]\bigr); \tag{27.4.44}$$

(b) To estimate terms (27.4.36)–(27.4.38) by the right-hand expression of (25.4.45); and

(c) To accommodate Dirac term in both upper and lower estimates.

Tasks (a), (b) are easy and we leave it to the reader (cf. arguments of Subsection 25.4.3); we use that after rescaling effective magnetic field intensity becomes $O(\alpha Z)$ in the zone $\{x : \ell(x) \asymp Z^{-\frac{1}{3}}\}$ due to already established estimates to A.

To fulfill task (c) observe that in the upper estimate we already have term

$$-\frac{1}{2}\operatorname{tr}\iint |x-y|^{-1} e_N(x,y)e_N^\dagger(x,y)\,dxdy. \tag{27.4.45}$$

On the other hand, in virtue of Theorem 26.A.2 we replace in the lower estimate term $-C\int \rho_\Psi^{\frac{4}{3}}(x)\,dx$ by (27.4.6) with $O(Z^{\frac{5}{3}-\delta})$ error (again we leave easy details to the reader).

One can prove by the same arguments as as in the non-magnetic case that for $\alpha Z \le \kappa^*$ it is $\mathsf{Dirac} + O(Z^{\frac{5}{3}-\delta})$. ☐

Finally, combining arguments sketched in the proof of Theorem 27.4.4 with the improved estimate of (27.4.43) (see Theorem 27.3.24(ii)) we arrive to

Theorem 27.4.5. *Let assumptions* (27.4.8) *and* (27.4.10) *be fulfilled, and let* $\alpha \le Z^{-\frac{10}{9}}|\log Z|^{-\frac{1}{3}}$. *Then*

$$\mathsf{E}_N^* = \mathcal{E}_N^{\mathsf{TF}} + \sum_{1\le m\le M} 2Z_m^2 S(\alpha Z_m) + \mathsf{Dirac} + \mathsf{Schwinger} + O\bigl(\alpha|\log(\alpha Z)|^{\frac{1}{3}}Z^{\frac{25}{9}} + Z^{\frac{5}{3}-\delta} + \alpha b^{-3}Z^2\bigr) \tag{27.4.46}$$

where Dirac *and* $\mathsf{Schwinger}$ *are* Dirac *and* Schwinger correction terms *defined exactly as in non-magnetic case by* (25.1.29) *and* (25.1.30) *respectively.*

27.4.5 Free Nuclei Model

Consider now free nuclei model (see Subsubsection *25.4.4.2). Estimates for Distance between Nuclei in the Free Nuclei Model*).

Theorem 27.4.6. *Let us consider $\mathsf{y}_m = \mathsf{y}_m^*$ minimizing the full energy*

$$\widehat{\mathsf{E}}_N^* := \mathsf{E}_N^* + \sum_{1\le m<m'\le M} Z_m Z_{m'} |\mathsf{y}_m - \mathsf{y}_{m'}|^{-1}. \tag{27.4.47}$$

Assume that

$$Z_m \asymp N \qquad \forall m = 1, \dots, M. \tag{27.4.48}$$

Then

$$b \ge \min\bigl(Z^{-\frac{5}{21}+\delta},\, Z^{-\frac{5}{21}}(\alpha Z)^{-\delta},\, \alpha^{-\frac{1}{4}} Z^{-\frac{1}{2}}\bigr) \tag{27.4.49}$$

and in the remainder estimates in (27.4.40) *and* (27.4.46) *one can skip b-connected terms; so we arrive to*

$$\mathsf{E}_N^* = \mathcal{E}_N^{\mathsf{TF}} + \sum_{1\le m\le M} 2Z_m^2 S(\alpha Z_m) + O\bigl(\alpha |\log(\alpha Z)|^{\frac{1}{3}} Z^{\frac{25}{9}} + Z^{\frac{5}{3}}\bigr) \tag{27.4.50}$$

and

$$\mathsf{E}_N^* = \mathcal{E}_N^{\mathsf{TF}} + \sum_{1\le m\le M} 2Z_m^2 S(\alpha Z_m) + \mathsf{Dirac} + \mathsf{Schwinger} + \\ O\bigl(\alpha |\log(\alpha Z)|^{\frac{1}{3}} Z^{\frac{25}{9}} + Z^{\frac{5}{3}-\delta}\bigr) \tag{27.4.51}$$

respectively and also the same asymptotics with $\widehat{\mathsf{E}}_N^*$ and $\widehat{\mathcal{E}}_N^{\mathsf{TF}}$ instead of E_N^* and $\mathcal{E}_N^{\mathsf{TF}}$.

Proof. Optimization with respect to $\mathsf{y}_1, \dots, \mathsf{y}_M$ implies

$$\mathsf{E}^* + \sum_{1\le m<m'\le M} \frac{Z_m Z_{m'}}{|\mathsf{y}_m - \mathsf{y}_{m'}|} < \sum_{1\le m\le M} \mathsf{E}_m^* \tag{27.4.52}$$

where $\mathsf{E}^* = \mathsf{E}^*(\mathsf{y}_1, \dots, \mathsf{y}_M; Z_1, \dots, Z_m, N)$ and $\mathsf{E}_m^* = \mathsf{E}^*(\mathsf{y}_m, Z_m)$ are calculated for separate atoms. In virtue of Theorem 27.4.3

$$\mathcal{E}^{\mathsf{TF}} + \sum_{1\le m<m'\le M} \frac{Z_m Z_{m'}}{|\mathsf{x}_m - \mathsf{x}_{m'}|} - \sum_{1\le m\le M} \mathcal{E}_m^{\mathsf{TF}} \le \\ C\alpha |\log(\alpha Z)|^{\frac{1}{3}} Z^{\frac{25}{9}} + Z^{\frac{5}{3}} + C\alpha b^{-3} Z^2. \tag{27.4.53}$$

However due to the strong non-binding theorem in Thomas-Fermi theory the left-hand expression is $\gtrsim b^{-7}$ for $b \geq Z^{-\frac{1}{3}}$ and therefore (27.4.53) implies

$$b \gtrsim \min\bigl(Z^{-\frac{5}{21}},\ \alpha^{-\frac{1}{7}}|\log(\alpha Z)|^{-\frac{1}{21}}Z^{-\frac{25}{63}},\ \alpha^{-\frac{1}{4}}Z^{-\frac{1}{2}}\bigr)$$

where the third expression is larger than the second one for sure. Unfortunately, for $\alpha \geq Z^{-\frac{10}{9}-\delta'}$ it is not as good as we claimed in (27.4.49). Still this estimate implies both (27.4.50) and (27.4.51).

To prove estimate (27.4.49) we observe that $b \gg Z^{-\frac{2}{7}}$ [19] and then we employ arguments used in the proof of Proposition 26.8.12 and prove that

$$|\operatorname{Tr}^-(H_{A,W}+\mu) - \sum_{1\leq m\leq M} \operatorname{Tr}^-(H_{A,W_m}+\mu) - \int \Bigl(\mathsf{Weyl}(H_{A,W}+\mu;\,x) - \sum_{1\leq m\leq M} \mathsf{Weyl}(H_{A,W_m}+\mu;\,x)\Bigr)\,dx| \leq CZ^{\frac{5}{3}}\bigl(Z^{-\delta}+(\alpha Z)^{\delta}\bigr),$$

where A be a minimizer for "molecular" expression (27.4.45) and W_m are atomic potentials. The same estimate holds if we replace $\operatorname{Tr}^-(H_{A,W_m}+\mu)$ by $\operatorname{Tr}^-(H_{A_m,W_m}+\mu)$ with $A_m = A\phi(b^{-1}|x-\mathsf{y}_m|)$ with $\phi \in \mathscr{C}_0^\infty(B(0,\frac{1}{3}))$, equal 1 in $B(0,\frac{1}{4})$. We leave an easy proof to the reader.

Then using the lower estimate for $\inf\operatorname{Spec}_{\mathfrak{H}}(\mathsf{H})$ and upper estimates for both $\inf\operatorname{Spec}_{\mathfrak{H}_m}(\mathsf{H}_m)$ through $\operatorname{Tr}^-(H_{A,W}+\mu)$ <u>and</u> $\operatorname{Tr}^-(H_{A_m,W_m}+\mu')$ respectively (where H_m are associated with H_{A_m,W_m}) we arrive to

$$\inf\operatorname{Spec}_{\mathfrak{H}}(\mathsf{H}) \geq \sum_{1\leq m\leq M} \inf\operatorname{Spec}_{\mathfrak{H}_m}(\mathsf{H}_m) + \mathcal{E}^{\mathsf{TF}} - \sum_{1\leq m\leq M}\mathcal{E}^{\mathsf{TF}}_m - CZ^{\frac{5}{3}}\bigl(Z^{-\delta}+(\alpha Z)^{\delta}\bigr)$$

and therefore

$$\mathsf{E}_A \geq \sum_{1\leq m\leq M}\mathsf{E}_{m,A_m} + \mathcal{E}^{\mathsf{TF}} - \sum_{1\leq m\leq M}\mathcal{E}^{\mathsf{TF}}_m - CZ^{\frac{5}{3}}\bigl(Z^{-\delta}+(\alpha Z)^{\delta}\bigr) - C\alpha b^{-3}Z^2, \tag{27.4.54}$$

where the last term is due to replacement of $\frac{1}{\alpha}\int|\nabla\times A|^2\,dx$ by "atomized" expressions $\sum_{1\leq m\leq M}\frac{1}{\alpha}\int|\nabla\times A_m|^2\,dx$.

[19] There is no binding with $b \leq Z^{-\frac{1}{3}}$ because remainder estimate is (better than) CZ^2 and binding energy excess is $\asymp Z^{\frac{7}{3}}$.

The last inequality (27.4.54) then obviously holds with A_m replaced by optimizers for "atomic" expressions (27.4.45) and *now* strong non-binding theorem implies that

$$b^{-7} \le CZ^{\frac{5}{3}}\bigl(Z^{-\delta} + (\alpha Z)^{\delta}\bigr) + C\alpha b^{-3}Z^2$$

which implies (27.4.49) where we change $\delta > 0$ as needed. □

27.5 Miscellaneous Problems

Recall that in our analysis in Sections 25.5 and 25.6 the crucial role was played by an estimate of $\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}}, \rho_\Psi - \rho^{\mathsf{TF}})$ and since what we have now (see Theorem 27.4.4) is (almost) as good as we had then, all arguments of these Sections still work with the minimal modifications. We leave most of the easy details to the reader but we need to deal with different magnetic fields for different N.

27.5.1 Excessive Negative Charge

Theorem 27.5.1 [20]**.** *Let condition* (27.4.48) *be fulfilled.*

(i) In the framework of the fixed nuclei model let us assume that $\mathsf{I}_N^* := \mathsf{E}_{N-1}^* - \mathsf{E}_N^* > 0$. *Then*

$$(N-Z)_+ \le CZ^{\frac{5}{7}}\begin{cases} 1 & \text{if } a \le Z^{-\frac{1}{3}},\\ Z^{-\delta} + (aZ^{\frac{1}{3}})^{-\delta} + (\alpha Z)^{\delta} & \text{if } a \ge Z^{-\frac{1}{3}}.\end{cases} \tag{27.5.1}$$

(ii) In particular, for a single atom and for molecule with $a \ge Z^{-\frac{1}{3}+\delta}$

$$(N-Z)_+ \le Z^{\frac{5}{7}}\bigl(Z^{-\delta} + (\alpha Z)^{\delta}\bigr). \tag{27.5.2}$$

(iii) In the framework of the free nuclei model let us assume that $\widehat{\mathsf{I}}_N^* := \widehat{\mathsf{E}}_{N-1}^* - \widehat{\mathsf{E}}_N^* > 0$. *Then estimate* (27.5.2) *holds.*

Proof. The proof follows the proof of Theorem 25.5.2; since it is not specific to the case where there is no magnetic field, we find that $(N-Z)_+ \le Q^{\frac{3}{7}}$, where Q is an estimate for $\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}}, \rho_\Psi - \rho^{\mathsf{TF}})$, which we established

[20] Cf. Theorem 25.5.2.

already; recall that the equivalence $\rho^{\mathsf{TF}} \asymp \ell^{-6}$ for $\ell \gtrsim Z^{-\frac{1}{3}}$ also plays an important role.

Here we pick up $A = A_N$ [21] and conclude that

$$\mathsf{I}_N(A) \coloneqq \mathsf{E}_{N-1}(A) - \mathsf{E}_N(A) \geq \mathsf{E}^*_{N-1} - \mathsf{E}^*_N > 0,$$

and then repeat arguments of the proof of Theorem 25.5.2.

We leave the remaining easy details to the reader. □

27.5.2 Estimates for iIonization Energy

Theorem 27.5.2 [22]**.** *Let condition* (27.4.48) *be fulfilled and let $N \geq Z - C_0 Z^{\frac{5}{7}}$. Then*

(i) In the framework of the fixed nuclei model

$$\mathsf{I}^*_N \leq CZ^{\frac{20}{21}}. \tag{27.5.3}$$

(ii) In the framework of the free nuclei model with $N \geq Z - C_0 Z^{\frac{5}{7}}\bigl(Z^{-\delta} + \alpha Z^{\delta}\bigr)$

$$\widehat{\mathsf{I}}^*_N \coloneqq \widehat{\mathsf{E}}^*_{N-1} - \widehat{\mathsf{E}}^*_{N-1} \leq Z^{\frac{20}{21}}\bigl(Z^{-\delta'} + (\alpha Z)^{\delta'}\bigr). \tag{27.5.4}$$

Proof. Recall that Theorem 25.5.3 was proven simultaneously with Theorem 25.5.2; we follow the same scheme here picking up $A = A_N$ [21]. Thus here and in the first part of the proof of Theorem 27.5.3 we estimate from above $\mathsf{I}^*_N(A)$.

Again the remaining easy details a left to the reader. □

Theorem 27.5.3 [23]**.** *Let condition* (27.4.48) *be fulfilled and let $N \leq Z - C_0 Z^{\frac{5}{7}}$. Then in the framework of the fixed nuclei model under assumption* (25.6.2)

$$(\mathsf{I}^*_N + \nu)_+ \leq C(Z-N)^{\frac{17}{18}} Z^{\frac{5}{18}} \begin{cases} 1 & \textit{if} \quad a \leq Z^{-\frac{1}{3}}, \\ Z^{-\delta} + (aZ^{\frac{1}{3}})^{-\delta} & \textit{if} \quad a \geq Z^{-\frac{1}{3}}. \end{cases} \tag{27.5.5}$$

[21] Exactly as in the analysis of free nuclei model we pick up $\underline{y}$ for N-electrons we pick now A for N electrons.

[22] Cf. Theorem 25.5.3.

[23] Cf. Theorem 25.6.3.

Proof. To estimate $\mathsf{I}_N^* + \nu$ from above we follow exactly the arguments of Subsection 25.6.1 to estimate $\mathsf{I}_N(A_N) \ge \mathsf{I}_N^*$. □

Problem 27.5.4. To prove the same estimate for $(\mathsf{I}_N^* + \nu)_-$.

Remark 27.5.5. To estimate $\mathsf{I}_N^* + \nu$ from below we need to pick up $A = A_{N-1}$ rather than $A = A_N$; then

$$\mathsf{I}_N(A) = \mathsf{E}_{N-1}(A) - \mathsf{E}_N(A) \le \mathsf{E}_{N-1}^* - \mathsf{E}_N^* = \mathsf{I}_N^*$$

and we should follow the arguments of Subsection 25.6.2. However, in contrast to all other proofs of this Section, here we should use the spectral properties of $H_{A,W}$ (or at least an estimate from above for its lowest eigenvalue after localization to $\mathsf{supp}(\theta)$, while in all other results we need an estimate from below for the same lowest eigenvalue after localization to $\mathsf{supp}(\theta)$).

To estimate from above the lowest eigenvalue of $H_{A,W}$ we need some uniform (i.e. with constants which do not depend on N) smoothness estimates for A_{N-1} where A_{N-1} is the minimizer for $\mathsf{E}_{N-1}(A)$ as defined in Sections 27.4 and here (rather than as defined in Sections 27.2–27.3).

While (27.A.1) is an analogue of (27.2.14), it is still not the same, and while it implies some estimate, it is not even remotely as good as we achieved in Sections 27.2 and 27.3.

Sure ρ_Ψ is not very smooth either but it close to rather smooth ρ^{TF}; on the other hand, the minimizer A_N is an almost-minimizer for the one-particle trace problem studied Sections 27.2–27.3 but we don't know how close it to the minimizer (or one of the minimizers) of the latter problem.

27.5.3 Free Nuclei Model: Excessive Positive Charge

Theorem 27.5.6 [24]**.** *Let condition* (27.4.48) *be fulfilled. Then in the framework of free nuclei model with $M \ge 2$ the stable molecule does not exist unless*

$$Z - N \le Z^{\frac{5}{7}}\bigl(Z^{-\delta} + (\alpha Z)^{\delta}\bigr). \tag{27.5.6}$$

Proof. Again we just repeat the proof of Theorem 25.6.4; we leave all easy details to the reader. □

[24] Cf. Theorem 25.6.4.

27.A Appendices

27.A.1 Minimizers and Ground States

First, establish a conditional existence of the minimizer[25] and the corresponding ground state of the original problem:

Theorem 27.A.1. *Let $\alpha Z < \kappa^*$ and let $\mathsf{E}^*_N < \mathsf{E}^*_{N-1}$. Then there exist a minimizer $A = A_N$ for the original multiparticle problem and the corresponding ground state Ψ_N.*

Proof. We know that for $\alpha Z < \kappa^*$ (with $\kappa^* > 0$ which does not depend on Z or positions of the nuclei) $\mathsf{E}^*(A)$ is bounded from below; then $\|\nabla \times A'\|^2$ is bounded from above for a near-minimizer A' (but constants do depend on Z and $(\kappa^* - \alpha Z)$ here). On the other hand, for $A' \in \mathscr{C}_0^\infty$ and $\mathsf{E}_N(A') < \mathsf{E}_{N-1}(A')$ there exists a ground state $\Psi_N(A')$.

Therefore if $A_{(k)} \in \mathscr{C}_0^\infty$ is a minimizing sequence for $\mathsf{E}_N(A)$ we have also a sequence $\Psi_N(A_{(k)})$ with $\|\Psi_N(A_{(k)})\| = 1$. Going if necessary to the subsequence, we can assume that $A_{(k)}$ converges weakly in $\mathscr{H}^1$ and strongly in $\mathscr{L}^p_{\mathsf{loc}}$ for any $p < 6$; let A be its limit.

One can prove easily that $\Psi_N(A_{(k)})$ converge weakly in $\mathscr{H}^1$ and strongly in $\mathscr{L}^2$ to Ψ and

$$(\mathsf{H}_{A,V}\Psi, \Psi) = \lim_{k\to\infty} (\mathsf{H}_{A_{(k)},V}\Psi_N(A_{(k)}), \Psi_N(A_{(k)})),$$

and then

$$(\mathsf{H}_{A,V}\Psi, \Psi) + \frac{1}{\alpha} = \lim_{k\to\infty} \mathsf{E}_N(A_{(k)}),$$

which is E^*_N since $A_{(k)}$ is a minimizing sequence and then Ψ must be a ground state. □

Now in this framework we establish properties of the minimizer and the ground state:

Proposition 27.A.2 [26]**.** *Let $\Psi = \Psi_N$ and $A = A_N$ be a ground state and minimizer with energy $\mathsf{E}^*_N < \mathsf{E}^*_{N-1}$.*

(i) $\Psi \in \mathscr{C}^1$ and $\Psi = O(e^{-\epsilon|\underline{x}|})$ as $|\underline{x}| \to \infty$.

[25] We do not know if it is unique.
[26] Cf. Proposition 26.A.7.

(ii) $A \in \mathscr{C}^1$ *and* $A = O(|x|^{-2})$, $\nabla \times A = O(|x|^{-3})$ *as* $|x| \to \infty$.

(iii) Let $N < Z$. *Then* $V_\Psi - V \in \mathscr{C}^1$ *and* $V_\Psi = (Z-N)|x|^{-1} + O(|x|^{-2})$, $\nabla V_\Psi = -(Z-N)x|x|^{-3} + O(|x|^{-3})$ *as* $|x| \to \infty$.

Proof. An obvious proof, using also an equation

$$\frac{2}{\alpha}\Delta A_j = \\ -2N\,\mathrm{Re}\,\mathrm{tr}\int \Psi^\dagger(x,x_2,\ldots,x_N)\sigma_j(D-A)_x\cdot\boldsymbol{\sigma}\Psi(x,x_2,\ldots,x_N)\,dx_2\cdots dx_N, \tag{27.A.1}$$

is left to the reader. This equation is similar to (27.2.14) and is also derived from variational principles, its right-hand expression is $\frac{\delta\Lambda}{\delta A}$ where Λ is the lowest eigenvalue of $\mathsf{H}_{A,V}$ on Fock' space.

27.A.2 Zhislin's Theorem

Theorem 27.A.3 (Zhislin's theorem) [27]**.** $\mathsf{E}^*_{N+1} < \mathsf{E}^*_N$ *if* $N < Z$.

Proof. An easy proof repeating with obvious modifications proof of Theorem 26.A.8 is left to the reader. □

27.A.3 L. Erdös–J. P. Solovej's Lemma

We reproduce here Lemma 2.1 from L. Erdös, J. P. Solovej [1].

Lemma 27.A.4. *There is a positive universal constant* κ^* *such that for any* Z,α *with* $Z\alpha \le \kappa^*$ *we have*

$$\inf_N \inf_A H_{A,V} \ge -CZ^{\frac{7}{3}}\delta^{1/2} - Z^{\frac{2}{3}}\delta^{-2}$$

if $CZ^{-\frac{2}{3}} \le \delta \le C_1$ *with a sufficiently large constant* C.

Proof. Consider a pair of smooth functions θ_0 and θ_1, such that $\theta_0^2 + \theta_1^2 = 1$, $\mathrm{supp}(\theta_1) \subset B(0,2r)$, $\theta_1 = 1$ on $B(0,r)$, and $|\nabla\theta_0|$, $|\nabla\theta_1| \le Cr^{-1}$ with $r = \delta Z^{-\frac{1}{3}}$.

[27] Cf. Theorem 26.A.8.

Let $\tilde\chi_0$ be a smooth cutoff function, supported on $B(0,3r)$ such that $|\nabla\tilde\chi_0|\le Cr^{-1}$ and $\tilde\chi_0=1$ on $B(0,2r)$. Let $\bar A$ be an average of A over $B(0,3r)$. Let $A_0:=(A-\bar A)\tilde\chi_0$, $B_0:=\nabla\times A_0$; then

$$\nabla\otimes A_0=\tilde\chi_0\nabla\otimes A+(A-\bar A)\otimes\nabla\tilde\chi_0.$$

Clearly

$$\int_{\mathbb{R}^3} B_0^2\,dx\le\int_{\mathbb{R}^3}|\nabla\otimes A_0|^2\,dx\le 2\int_{\mathbb{R}^3}\tilde\chi_0^2|\nabla\otimes A|^2\,dx+Cr^{-2}\int_{B(0,3r)}(A-\bar A)^2\,dx\\ \le C_1\int_{B(0,3r)}|\nabla\otimes A|^2\,dx$$

for some universal constant C_1, where in the last step we used the Poincaré inequality. Let φ be a real phase such that $\nabla\varphi=\bar A$. Since $\tilde\chi_0\equiv 1$ on the support of θ_1, we have

$$\theta_1H_{A,0}\theta_1=\theta_1e^{-i\varphi}H_{A-\bar A,0}e^{i\varphi}\theta_1=\theta_1e^{-i\varphi}H_{A_0,V}e^{i\varphi}\theta_1.$$

After these localizations, we have

$$H^1_{N,Z;A}:=\\ \sum_{j=1}^N\Bigl[\theta_1\Bigl(H_{A,0}-\frac{Z}{|x|}-\bigl(|\nabla\theta_0|^2+|\nabla\theta_1|^2\bigr)\theta_1\Bigr]_j+\frac{1}{\alpha}\int_{B(0,3r)}|\nabla\otimes A|^2\,dx\\ \ge\sum_{j=1}^N\Bigl[\theta_1e^{-i\varphi}\bigl(H_{A_0,0}-W(x)\bigr)e^{i\varphi}\theta_1\Bigr]_j+\frac{1}{2C_1\alpha}\int B_0^2\,dx \tag{27.A.2}$$

with

$$W(x)=\Bigl[\frac{Z}{|x|}+Cr^{-2}\Bigr]\mathbf{1}(|x|\le 2r),$$

where $\mathbf{1}(X)$ is a characteristic function of X.

Now we use the "running energy scale" argument in E. Lieb, M. Loss, M. and J. Solovej [1].

$$\sum_{j=1}^N\Bigl[\theta_1e^{-i\varphi}\bigl[H_{A',0}-W\bigr]e^{i\varphi}\theta_1\Bigr]_j\ge-\int_0^\infty \mathsf{N}_{-e}(H_{A',0}-W)\,de\\ \ge-\int_0^\mu \mathsf{N}_{-e}(H_{A',0}-W)\,de-\int_\mu^\infty \mathsf{N}_0\bigl(\frac{\mu}{e}H_{A',0}-W+e\bigr)\,de\\ \ge-\int_0^\mu \mathsf{N}_{-e}(H_{A',0}-W)\,de-\int_\mu^\infty \mathsf{N}_0\Bigl(H_{A',0}-\frac{e}{\mu}W+\frac{e^2}{\mu}\Bigr)\,de, \tag{27.A.3}$$

where $\mathsf{N}_{-e}(H)$ denotes the number of eigenvalues of a self-adjoint operator H below $-e$.

In the first term we use the bound $H_{A_0,0}\ge (D-A_0)^2-|B_0|$ and the CLR (i.e. Cwikel-Lieb-Rozenblum) bound:

$$\begin{aligned}
&\int_0^\mu \mathsf{N}_{-e}(H_{A_0,0}-W)\,de \le C\int_0^\mu de\int_{\mathbb{R}^3}(W+|B_0|-e)_+^{\frac{3}{2}}\,dx \qquad (27.A.4)\\
&\le C\int_0^\mu de\int_{\mathbb{R}^3}(W-e/2)_+^{\frac{3}{2}}\,dx + C\int_0^\mu de\int_{\mathbb{R}^3}(|B_0|-e^2/2\mu)_+^{\frac{3}{2}}\,dx\\
&\le C\int_{\mathbb{R}^3}W^{\frac{5}{2}}\,dx + C\mu^{\frac{1}{2}}\int_{\mathbb{R}^3}B_0^2\,dx = CZ^{\frac{5}{2}}r^{\frac{1}{2}}+Cr^{-2}+C\mu^{\frac{1}{2}}\int_{\mathbb{R}^3}B_0^2\,dx.
\end{aligned}$$

In the second term of (27.A.3) we use

$$\begin{aligned}
H_{A_0,0}-\frac{e}{\mu}W \ge \frac{1}{2}\bigl[(D-A_0)^2-\frac{2eZ}{\mu|x|}\mathbf{1}(|x|\le 2r)\bigr]&\\
+\frac{1}{2}(D-A_0)^2-|B_0|-\frac{Ce}{\mu r^2}\mathbf{1}(|x|\le 2r)&,
\end{aligned}$$

and that

$$(D-A_0)^2-\frac{2eZ}{\mu|x|}\mathbf{1}(|x|\le 2r)\ge (D-A_0)^2-\frac{4eZ}{\mu|x|}\ge -(\frac{2eZ}{\mu})^2$$

i.e.

$$H_{A_0,0}-\frac{e}{\mu}W\ge \frac{1}{2}(D-A_0)^2-2(\frac{eZ}{\mu})^2-|B_0|-\frac{Ce}{\mu r^2}\mathbf{1}(|x|\le 2r).$$

Let $\mu=4Z^2$, then using $Ce/\mu r^2\le e^2/4\mu$ for $\mu\le e$ (i.e. $C\le(\delta Z^{2/3})^2$), we get

$$\begin{aligned}
&\int_\mu^\infty \mathsf{N}_0\bigl(H_{A_0,0}-\frac{e}{\mu}W+\frac{e^2}{\mu}\bigr)\,de \qquad (27.A.5)\\
&\le \int_\mu^\infty \mathsf{N}_0\bigl(\frac{1}{2}(D-A_0)^2-|B_0|+\frac{e^2}{4\mu}\bigr)\,de\le C\int_0^\mu de\int_{\mathbb{R}^3}(|B_0|-e^2/4\mu)_+^{3/2}\,dx\\
&\le C\mu^{\frac{1}{2}}\int_{\mathbb{R}^3}B_0^2\,dx.
\end{aligned}$$

Note that if $Z\alpha\le\kappa^*$ with some sufficiently small universal constant κ^*, then (27.A.5) can be controlled by the corresponding term in (27.A.2). Combining the estimates (27.A.2), (27.A.3), (27.A.4) and (27.A.5), we obtain

$$H_{A,V} \geq -CZ^{\frac{5}{2}} r^{\frac{1}{2}} - Cr^{-2}$$

and lemma follows. □

Comments

The problem was considered first in several papers of L. Erdös, J. P. Solovej [1] and L. Erdös, S. Fournais, J. P. Solovej [1, 3, 4].

The same problem in the relativistic case was considered in L. Erdös, S. Fournais, J. P. Solovej [2] (under assumption preventing relativistic instability).

Chapter 28

The Case of Combined Magnetic Field

28.1 Introduction

In this Chapter instead of the Schrödinger operator without magnetic field as in Chapter 25, or with a constant magnetic field as in Chapter 26, or with a self-generated magnetic field as in Chapter 27 we consider the Schrödinger operator (27.1.1) with unknown magnetic field A, but then we add to the ground state energy of the atom (or molecule) the energy of the self-generated magnetic field (see selected term in (28.1.1) thus arriving to

$$\mathsf{E}(A) = \inf \operatorname{Spec}(\mathsf{H}_{A,V}) + \underbrace{\alpha^{-1}\int |\nabla \times (A - A^0)|^2\, dx} \tag{28.1.1}$$

where $A^0 = \frac{1}{2}B(-x_2, x_1, 0)$ is a constant *external magnetic field*.

Then finally

$$\mathsf{E}^* = \inf_{A - A^0 \in \mathscr{H}^1_0} \mathsf{E}(A), \tag{28.1.2}$$

defines a ground state energy with a *combined magnetic field* A while $A' := A - A^0$ is a *self-generated magnetic field*.

Note that

$$\int |\nabla \times (A - A^0)|^2\, dx = \int \bigl(|\nabla \times A|^2 - |\nabla \times A^0|^2\bigr)\, dx \tag{28.1.3}$$

which seems to be a more "physical" definition.

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28.1.1 Plan of the Chapter

First of all, we are lacking so far a *semiclassical local theory* and we are developing it in Sections 28.2–28.4, where we consider a one-particle quantum Hamiltonian (28.2.1) with the external constant magnetic field A^0 of intensity β, $h \ll 1$ and a self-generated magnetic field $(A - A^0)$. Here theory significantly depends if $\beta h \lesssim 1$ or $\beta h \gtrsim 1$ as it was in the case without a self-generated magnetic field.

While Section 28.2 is preparatory and rather functional-analytical, Sections 28.3 and 28.4 are microlocal; they cover cases $\beta h \lesssim 1$ and $\beta h \gtrsim 1$ respectively. These three sections are similar to a single Section 27.2. However in Sections 28.3 and 28.4 various non-degeneracy assumptions play a very significant role, especially for large β.

Then in Section 28.5 we consider a global theory if a potential has Coulomb singularities and (in some statements) behaves like (magnetic) Thomas-Fermi potential both near singularities and far from them.

Finally, in Section 28.6 we apply these results to our original problem of the ground state energy so far assuming that the number of nuclei is 1. One can recover the same results if $M \geq 2$ but the external magnetic field B is weak enough. No surprise that the theory is different in the cases $B \leq Z^{\frac{4}{3}}$ and $Z^{\frac{4}{3}} \leq B \ll Z^3$ (see Chapter 25 where this difference appears). Since as $M = 1$ the strongest non-degeneracy assumption is surely achieved and as $M \geq 2$ much weaker non-degeneracy assumption is achieved in the border zone (see Chapter 25) our remainder estimates for large B significantly differ in the atomic and molecular cases.

In Appendix 28.A we first generalize Lieb-Loss-Solovej estimate to the case of the combined magnetic field (which is necessary if $\beta h \gtrsim 1$), then establish electrostatic inequality in the current settings and finally study very special pointwise spectral expressions for a Schrödinger operator in $\mathbb{R}^3$ with linear magnetic and scalar potentials (we considered such operators already in Section 16.6)

28.1.2 Unfinished Business

One can apply these results to estimates of the excessive positive and negative charges (the estimates for excessive positive charges, if $M \geq 2$ in the free nuclei framework) and estimates or asymptotics of the ionization energy in the same manner as we did it in Chapters 25–27; however there are no new ideas but rather tedious calculations and we leave it to those readers who decide to explore these topics, which is clearly serious task.

28.2 Local Semiclassical Trace Asymptotics: Preparation

28.2.1 Toy-Model

Let us consider operator (27.1.4)

$$H = H_{A,V} = \bigl((hD - A)\cdot \boldsymbol{\sigma}\bigr)^2 - V(x) \tag{28.2.1}$$

in $\mathbb{R}^3$ where A, V are real-valued functions and $V \in \mathscr{C}^{\frac{5}{2}}$, $A - A^0 \in \mathscr{H}^1_0$. Then operator $H_{A,V}$ is self-adjoint. We are interested in $\operatorname{Tr}^-(H_{A,V}) = \operatorname{Tr}^-(H^-_{A,V})$ (the sum of all negative eigenvalues of this operator). Let

$$\mathsf{E}^* = \mathsf{E}^*_\kappa := \inf_{A - A^0 \in \mathscr{H}^1_0} \mathsf{E}(A), \tag{28.2.2}$$

where

$$\mathsf{E}(A) = \mathsf{E}_\kappa(A) := \Bigl(\operatorname{Tr}^-(H_{A,V}) + \kappa^{-1}h^{-2}\int |\partial(A - A^0)|^2\,dx\Bigr) \tag{28.2.3}$$

with a matrix $\partial A = (\partial_i A_j)_{i,j=1,2,3}$. Recall that A^0 is a linear potential, $A^0(x) = \frac{1}{2}\beta(-x_2, x_1, 0)$. We consider rather separately cases

$$\beta h \lesssim 1 \qquad \text{and} \qquad \beta h \gtrsim 1 \tag{28.2.4$_{1,2}$}$$

of the *moderate* and *strong* external magnetic field.

To deal with the described problem we need to consider first a formal semiclassical approximation.

28.2.2 Formal Semiclassical Theory

Semiclassical Theory: $\beta h \lesssim 1$

Let us replace the trace expression $\operatorname{Tr}(H^-_{A,V}\psi)$ by its magnetic semiclassical approximation $-h^{-3}\int P_{Bh}(V)\psi\,dx$ where $B = |\nabla \times A|$ is a scalar intensity of the magnetic field and $P_*(.)$ is a pressure. Then $\mathsf{E}(A) \approx \mathcal{E}(A)$ with

$$\mathcal{E}(A) = \mathcal{E}_\kappa(A) := -h^{-3}\int P_{Bh}(V)\psi\,dx + \frac{1}{\kappa h^2}\int |\partial A'|^2\,dx. \tag{28.2.5}$$

Assuming that $|\partial A'| \ll \beta$, $A' = (A - A^0)$ we find out that

$$\begin{aligned}
(28.2.6)\quad & -h^{-3}\int P_{Bh}(V)\psi\,dx\\
&\approx -h^{-3}\int \Bigl(P_{\beta h}(V) - \partial_\beta P_{\beta h}(V)(B-\beta)\psi\Bigr)\,dx\\
&\approx -h^{-3}\int P_{\beta h}(V)\psi\,dx\\
&- h^{-3}\int \Bigl[\partial_{x_2}\bigl(\partial_\beta P_{\beta h}(V)\psi\bigr)\cdot A'_1 - \partial_{x_1}\bigl(\partial_\beta P_{\beta h}(V)\psi\bigr)\cdot A'_2\Bigr]\,dx,
\end{aligned}$$

where we used that

$$B \approx \beta - \partial_{x_2}A'_1 + \partial_{x_1}A'_2 \tag{28.2.7}$$

and integrated by parts. Then $\mathcal{E}(A) \approx \bar{\mathcal{E}}(A)$ with

$$\begin{aligned}
(28.2.8)\quad & \bar{\mathcal{E}}(A) = \bar{\mathcal{E}}_\kappa(A) := -h^{-3}\int P_{\beta h}(V)\psi\,dx\\
-h^{-3}&\int \Bigl[\partial_{x_2}\bigl(\partial_\beta P_{\beta h}(V)\psi\bigr)\cdot A'_1 - \partial_{x_1}\bigl(\partial_\beta P_{\beta h}(V)\psi\bigr)\cdot A'_2\Bigr]\,dx + \frac{1}{\kappa h^2}\int |\partial A'|^2\,dx
\end{aligned}$$

and replacing approximate equalities by exact ones and optimizing with respect to A' we arrive to

$$\begin{aligned}
(28.2.9)\quad \Delta A'_1 = -\frac{1}{2}\kappa h^{-1}\partial_{x_2}\bigl(\partial_\beta P_{\beta h}(V)\psi\bigr),\quad \Delta A'_2 = \frac{1}{2}\kappa h^{-1}\partial_{x_1}\bigl(\partial_\beta P_{\beta}(V)\psi\bigr),\\
\Delta A'_3 = 0
\end{aligned}$$

and

$$\mathcal{E}^*_\kappa := \inf_{A:\ A-A^0\in\mathscr{H}^1_0} \mathcal{E}_\kappa(A) \approx \bar{\mathcal{E}}^*_\kappa := \inf_{A:\ A-A^0\in\mathscr{H}^1_0} \bar{\mathcal{E}}_\kappa(A). \tag{28.2.10}$$

To justify our analysis we need to justify approximate equality

$$\begin{aligned}
(28.2.11)\quad & -h^{-3}\int P_{Bh}(V)\,dx + \frac{1}{\kappa h^2}\int |\partial A'|^2\,dx\\
\approx -h^{-3}&\int P_{\beta h}(V)\psi dx - h^{-3}\int \Bigl[\partial_\beta P_{\beta h}(V)\psi(-\partial_{x_2}A'_1 + \partial_{x_1}A'_2)\Bigr]\,dx +\\
&\frac{1}{\kappa h^2}\int |\partial A'|^2\,dx
\end{aligned}$$

and estimate an error when we minimize the right-hand expression instead of the left-hand one. To do this observe that (even without assumptions $Bh\lesssim 1$, $\beta h\lesssim 1$)

$$|P_{Bh}(V)-P_{\beta h}(V)-\partial_{\beta h}P_{\beta h}(V)\cdot (B-\beta)h|\le \\ C(B-\beta)^2h^2+C|B-\beta|^{\frac{3}{2}}\beta h^{\frac{5}{2}}. \tag{28.2.12}$$

Indeed, one can prove it easily recalling that

$$P_{\beta h}(V)=\varkappa_0\sum_{j\ge 0}(1-\frac{1}{2}\delta_{j0})(V-2j\beta h)_+^{\frac{3}{2}}\beta h \tag{28.2.13}$$

and considering cases $\beta h\gtrless 1$, $Bh\gtrless 1$, $|B-\beta|\gtrless \beta h$, analyzing different terms in (28.2.13) and observing that the last term in (28.2.12) appears only in the case $\beta h\lesssim 1$, $|B-\beta|\lesssim \beta$.

Then since $|B-\beta|\le |B'|$ (where $B'=|\partial(A-A^0)|$) we conclude that the left-hand expression of (28.2.11) is greater than

$$-h^{-3}\int P_{\beta h}(V)\psi dx - C\|B'\|\beta h^{-1}-C\|B'\|^{\frac{3}{2}}\beta h^{-\frac{1}{2}}+\kappa^{-1}h^{-2}\|B'\|^2,$$

where we used that

$$|\partial_{\beta h}P_{\beta h}(V)|\le C\beta h \qquad \text{if} \quad V\le c; \tag{28.2.14}$$

then a minimizer for the left-hand expression of (28.2.11) must satisfy

$$\|B'\|\le C\kappa\beta h \tag{28.2.15}$$

and one can observe easily that the same is true and for the minimizer for the right-hand expression as well.

Also observe that

$$B=\beta+\partial_{x_1}A'_2-\partial_{x_2}A'_1+O(\beta^{-1}|B'|^2). \tag{28.2.16}$$

Then for both minimizers the differences between the left-hand and right-hand expressions of (28.2.11) do not exceed $C\kappa^{\frac{5}{2}}\beta^{\frac{5}{2}}$ and therefore

$$|\mathcal{E}^*-\bar{\mathcal{E}}^*|\le C\kappa^{\frac{5}{2}}\beta^{\frac{5}{2}}. \tag{28.2.17}$$

One can calculate easily the minimizer for

$$-h^{-3}\int\Bigl[\partial_\beta P_{\beta h}(V)\psi(-\partial_{x_2}A'_1+\partial_{x_1}A'_2)\Bigr]\,dx+\frac{1}{\kappa h^2}\int|\partial A'|^2\,dx \tag{28.2.18}$$

and conclude that $A'_j=\kappa\beta h a_j$ with $a_3=0$ and

$$\Delta a_1=-(\beta h)^{-1}\partial x_2\partial_{\beta h}P_{\beta h}(V),\quad \Delta a_2=(\beta h)^{-1}\partial x_1\partial_{\beta h}P_{\beta h}(V) \tag{28.2.19}$$

and the minimum is negative and $O(\kappa\beta^2)$; we call it *correction term*; in fact, $\|\partial A'\|\asymp\kappa\beta h$ and the minimum is $\asymp-\kappa\beta^2$ in the generic case.

Then a minimum of the left-hand expression of (28.2.11) is equal to the minimum of the right-hand expression modulo $O(\kappa^{\frac{3}{2}}\beta^{\frac{5}{2}}h)$.

Remark 28.2.1. (i) One can improve this estimate under non-degeneracy assumptions (28.3.60) or (28.3.65). However even in the general case observe that

$$\begin{aligned}
&\mathcal{E}(A'')-\mathcal{E}(A')\\
&\ge -C\beta h^{-\frac{1}{2}}\|B'-B''\|^{\frac{3}{2}}-C\beta h^{-\frac{1}{2}}\|B'\|^{\frac{1}{2}}\cdot\|B'-B''\|+2\epsilon_0\kappa^{-1}h^{-2}\|\partial(A'-A'')\|^2\\
&\qquad\qquad\ge -C\kappa^2\beta^2 h+\epsilon_0\kappa^{-1}h^{-2}\|\partial(A'-A'')\|^2
\end{aligned}$$

if A' is the minimizer for $\bar{\mathcal{E}}$ and therefore since $\|B'\|\le C\kappa\beta h$ we conclude that

$$\mathcal{E}^*\ge\mathcal{E}(A')-C\kappa^2\beta^2 h \tag{28.2.20}$$

and

$$\|\partial(A'-A'')\|\le C\kappa^{\frac{3}{2}}\beta h^{\frac{1}{2}} \tag{28.2.21}$$

if A'' is an almost-minimizer for $\mathcal{E}(A'')$.

(ii) Observe, that picking up $A'=0$ and applying arguments of Chapter 18 we can derive an upper estimate

$$\mathsf{E}^*\le-\int P_{\beta h}(V)\psi\,dx+O(h^{-1}); \tag{28.2.22}$$

however this estimate is not sharp for $\kappa\beta^2\gg h^{-1}$ because $\mathcal{E}^*$ is less than the main term here with a gap $\asymp\kappa\beta^2$. For $\kappa\asymp 1$ it gives us a proper upper estimate only if $\beta\le h^{-\frac{1}{2}}$.

Therefore for $\kappa\beta^2\gg h^{-1}$ an upper estimate is not as trivial as in Chapter 26; in the future we pick up as A' a minimizer for $\bar{\mathcal{E}}(A)$ (mollified by x as this minimizer is not smooth enough).

Semiclassical Theory: $\beta h \gtrsim 1$

Consider $\beta h \ge 1$. Without any loss of the generality one can assume that $\|V\|_{\mathscr{L}^\infty} \le \beta h$ and $\|\partial A'\|_{\mathscr{L}^\infty} \le \frac{1}{2}\beta$. Then in the definition (28.2.13) of $P_{\beta h}(V)$ (etc) remains only term with $j = 0$:

$$P_{\beta h}(V) = \frac{1}{2}\varkappa_0 V_+^{\frac{3}{2}}\beta h, \tag{28.2.13$'$}$$

which leads to simplifications of $\mathcal{E}(A')$ and $\bar{\mathcal{E}}(A')$; both of them become

$$\frac{1}{2}\varkappa_0\beta h^{-2}\int V_+^{\frac{3}{2}}\psi\, dx + \frac{1}{2}\varkappa_0 h^{-2}\int V_+^{\frac{3}{2}}\bigl(\partial_{x_1}A'_2 - \partial_{x_2}A'_1\bigr)\psi\, dx + \kappa^{-1}h^{-2}\|\partial A'\|^2 \tag{28.2.8$'$}$$

modulo $O(\beta^{-1}h^{-2}\|B'\|^2)$ and equations to the minimizer become

$$\Delta A'_1 = -\frac{1}{2}\varkappa_0\kappa\partial_{x_2}\bigl(V_+^{\frac{3}{2}}\psi\bigr), \quad \Delta A'_2 = \frac{1}{2}\varkappa_0\kappa\partial_{x_1}\bigl(V_+^{\frac{3}{2}}\psi\bigr), \quad \Delta A'_3 = 0. \tag{28.2.9$'$}$$

Then $\|B'\| \asymp \kappa$ and a correction term is negative and $\asymp -\kappa h^{-2}$ in the generic case. An error $O(\beta^{-1}h^{-2}\|B'\|^2)$ becomes $O(\kappa\beta^{-1}h^{-2})$ (and thus not exceeding microlocal error $O(\beta)$).

28.2.3 Estimate from below

Basic Estimates

Let us estimate $\mathsf{E}(A)$ from below. First we need the following really simple

Proposition 28.2.2 [1]**.** *Consider operator $H_{A,V}$, defined on $\mathscr{H}^2(B(0,1)) \cap \mathscr{H}_0^1(B(0,1))$* [2]*. Let $V \in \mathscr{L}^4$.*

(i) Let $\beta h \le 1$. Then

$$\mathsf{E}^* \ge -Ch^{-3} \tag{28.2.23}$$

and either

$$\frac{1}{\kappa h^2}\int |\partial(A - A^0)|^2\, dx \le Ch^{-3} \tag{28.2.24}$$

or $\mathsf{E}(A) \ge ch^{-3}$.

[1] Cf. Proposition 27.2.1.

[2] I.e. on $\mathscr{H}^2(B(0,1))$ with the Dirichlet boundary conditions.

(ii) Let $\beta h\ge 1$. *Then*

$$\mathsf{E}^*\ge -C\beta h^{-2}-C\kappa^{\frac{1}{3}}\beta^{\frac{4}{3}}h^{-\frac{4}{3}} \tag{28.2.25}$$

and either

$$\frac{1}{\kappa h^2}\int |\partial(A-A^0)|^2\,dx\le C\beta h^{-2}+C\kappa^{\frac{1}{3}}\beta^{\frac{4}{3}}h^{-\frac{4}{3}} \tag{28.2.26}$$

or $\mathsf{E}(A)\ge C\beta h^{-2}+C\kappa^{\frac{1}{3}}\beta^{\frac{4}{3}}h^{-\frac{4}{3}}$.

(iii) Furthermore, let $\beta h\ge 1$ *and*

$$\kappa\beta h^2\le c. \tag{28.2.27}$$

Then

$$\mathsf{E}^*\ge -C\beta h^{-2} \tag{28.2.28}$$

and either

$$\frac{1}{\kappa h^2}\int |\partial(A-A^0)|^2\,dx\le C\beta h^{-2} \tag{28.2.29}$$

or $\mathsf{E}(A)\ge C\beta h^{-2}$.

Proof. Using estimate (28.A.2) [3)] we have

$$\mathsf{E}(A)\ge -C(1+\beta h)h^{-3}\\ -C\beta h^{-\frac{3}{2}}\Bigl(\int |\partial A'|^2\,dx\Bigr)^{\frac{1}{4}}-Ch^{-\frac{3}{2}}\Bigl(\int |\partial A'|^2\,dx\Bigr)^{\frac{3}{4}}+\frac{1}{\kappa h^2}\Bigl(\int |\partial A'|^2\,dx\Bigr), \tag{28.2.30}$$

which implies both Statements (i)–(ii) while Statement (iii) is a special case of Statement (ii). □

Remark 28.2.3. (i) Definitely we would prefer to have an estimate

$$\mathsf{E}(A)\ge -C(1+\beta h)h^{-3}\\ -Ch^{-2}\Bigl(\int |\partial A'|^2\,dx\Bigr)^{\frac{1}{2}}+\frac{1}{\kappa h^2}\Bigl(\int |\partial A'|^2\,dx\Bigr) \tag{28.2.31}$$

from the very beginning, but we cannot prove it without some smoothness conditions to A and they will be proven only later under the same assumption (28.2.27).

[3)] Magnetic Lieb–Thirring inequality (5) of E. H. Lieb, M. Loss, M. and J. P. Solovej [1]) would be sufficient for $\beta h\le 1$ but will lead to a worse estimate than we claim for $\beta h\ge 1$.

(ii) This assumption (28.2.27) in a bit stronger form $(28.2.27)^*$ will be required for our microlocal analysis in the next Section 28.3.

Remark 28.2.4. Using Proposition 28.2.2 one can prove easily the following:

(i) Proposition 27.2.2 (existence of the minimizer) remains valid;

(ii) As in Remark 27.2.3 we do not know if the minimizer is unique. From now on until further notice let A be a minimizer. We also assume that V is sufficiently smooth ($V \in \mathscr{C}^{2+\delta}$). This is be the case for magnetic Thomas-Fermi potential for sure.

(iii) Proposition 27.2.4 (namely, equation (27.2.14) to a minimizer) remains valid for both A and $A' = A - A^0$.

Proposition 28.2.5 [4]**.** *(i) Let $\beta h \le 1$ and $0 < \kappa \le (1-\epsilon_0)\kappa^*$. Assume that*

$$\mathsf{E}^*(\kappa^*, \beta, h) \ge \mathcal{E} - CM, \tag{28.2.32}$$

$$\mathsf{E}^*(\kappa, \beta, h) \le \mathcal{E} + CM \tag{28.2.33}$$

with the same number $\mathcal{E}$ and with $M \ge Ch^{-1} + C\kappa^*\beta^2$. Then

$$\int |\partial A'|^2\, dx \le C_1 \kappa h^2 M; \tag{28.2.34}$$

(ii) Let $\beta h \ge 1$ and $\kappa^*\beta h \le c$, $0 < \kappa \le (1-\epsilon_0)\kappa^*$. Assume that (28.2.32)–(28.2.33) *are fulfilled with the same number $\mathcal{E}$ and with $M \ge C\beta + C\kappa^* h^{-2}$. Then estimate also* (28.2.34) *holds.*

Proof. Proof obviously follows the proof of Proposition 27.2.5. □

Estimates to a Minimizer: $\beta h \lesssim 1$

Consider first the simpler case $\beta h \le 1$.

[4] Cf. Proposition 27.2.5.

Proposition 28.2.6. *Let $\beta h \le 1$. Then*

$$|e(x,y,\tau)| \le C\bigl(1+\mu^{\frac{1}{2}}h^{\frac{1}{2}}\bigr)h^{-3} \tag{28.2.35}$$

and

$$|((hD-A)_x\cdot\boldsymbol{\sigma})e(x,y,\tau)| \le C\bigl(1+\mu^{\frac{1}{2}}h^{\frac{1}{2}}\bigr)h^{-3}, \tag{28.2.36}$$

where

$$\mu = \|\partial A'\|_\infty. \tag{28.2.37}$$

Proof. Without any loss of the generality one can assume that $\mu h \ge 1$. Consider $\mu^{-\frac{1}{2}}h^{\frac{1}{2}}$-element in $\mathbb{R}^3_x$. Without any loss of the generality one can assume that $A^0(z)=A(z)=0$ in its center z.

Since both operators $E(\tau)$ and $((hD-A)_x\cdot\boldsymbol{\sigma})E(\tau)$ have their operator norms bounded by c in $\mathscr{L}^2$, one can prove easily that both operators $\phi D^\alpha E(\tau)$ and $\phi D^\alpha((hD-A)_x\cdot\boldsymbol{\sigma})E(\tau)$ have their operator norms bounded by $C\zeta^{|\alpha|}$ with $\zeta=\mu^{\frac{1}{2}}h^{-\frac{1}{2}}$ if $\alpha\in\{0,1\}^3$ and ϕ is supported in the mentioned element.

Then operator norms of both operators $\gamma_x E(\tau)$ and $\gamma_x((hD-A)_x\cdot\boldsymbol{\sigma})E(\tau)$ from $\mathscr{L}^2$ to $\mathbb{C}^q$ do not exceed $C_0\zeta_1\zeta_3^{\frac{1}{2}}$ and therefore the same is true for adjoint operators; here γ_z is operator of restriction to $x=z$.

Since $E(\tau)^*=E(\tau)^2=E(\tau)$ we conclude that the left-hand expressions in (28.2.35) and (28.2.36) do not exceed $C\zeta^3$, which is exactly the right-hand expression in both of them.

Then from equation (27.2.14), which remains valid (see Remark 28.2.4(iii)) we conclude that

$$\|\Delta A'\|_{\mathscr{L}^\infty} \le C\kappa\bigl(1+\mu^{\frac{1}{2}}h^{\frac{1}{2}}\bigr)h^{-1} \tag{28.2.38}$$

and therefore

$$\|\partial^2 A'\|_{\mathscr{L}^\infty} \le C\kappa|\log h|\bigl(1+\mu^{\frac{1}{2}}h^{\frac{1}{2}}\bigr)h^{-1}. \tag{28.2.39}$$

Further, combining (28.2.39) with (28.2.24), the standard inequality $\|\partial A'\|_{\mathscr{L}^\infty}\le \|\partial^2 A'\|^{\frac{3}{5}}_{\mathscr{L}^\infty}\cdot\|\partial A'\|^{\frac{2}{5}}$ and (28.2.37), we conclude that

$$\mu \le C(\kappa|\log h|)^{\frac{4}{5}}\bigl(1+\mu^{\frac{1}{2}}h^{\frac{1}{2}}\bigr)^{\frac{4}{5}}h^{-\frac{4}{5}}$$

and therefore $\mu h \ll 1$. Then

$$\|\partial A'\|_{\mathscr{L}^\infty} \le C(\kappa|\log h|)^{\frac{4}{5}}h^{-\frac{4}{5}} \tag{28.2.40}$$

and therefore due to (28.2.39)

$$\|\partial A'\|_{\mathscr{L}^\infty} \le C\kappa |\log h| h^{-1} \tag{28.2.41}$$

(where for a sake of simplicity we slightly increase power of logarithm) thus arriving to

Proposition 28.2.7. *Let $\beta h \le 1$ and $\kappa \le \kappa^*$. Let A be a minimizer. Then estimates* (28.2.40) *and* (28.2.41) *hold.*

Furthermore, the standard scaling arguments applied to the results of Section 27.2 imply that in fact the left-hand expressions of estimates (28.2.36) and (28.2.24) do not exceed $C(1+\beta+\mu)h^{-2}$ and $C(1+\beta+\mu)^2h^{-1}$ respectively.

Therefore $\|\partial^2 A'\|_{\mathscr{L}^\infty}$ does not exceed $C\kappa|\log h|(1+\beta+\mu)$ and $\|\partial A'\|$ does not exceed $C\kappa^{\frac{1}{2}}(1+\beta+\mu)h^{\frac{1}{2}}$, and then $\mu \le C(\kappa|\log h|)^{\frac{4}{5}}(1+\beta+\mu)^{\frac{4}{5}}h^{\frac{1}{5}}$ which implies $\mu \le C(\kappa|\log h|)^{\frac{4}{5}}(1+\beta)^{\frac{4}{5}}h^{\frac{1}{5}}$ and finally we arrive to

Proposition 28.2.8. *Let $\beta h \le 1$ and $\kappa \le \kappa^*$. Then*

$$\|\partial A'\|_{\mathscr{L}^\infty} \le C(\kappa|\log h|)^{\frac{4}{5}}(1+\beta)^{\frac{4}{5}}h^{\frac{1}{5}} \tag{28.2.42}$$

and

$$\|\partial^2 A'\|_{\mathscr{L}^\infty} \le C\kappa|\log h|(1+\beta). \tag{28.2.43}$$

Estimates to a Minimizer: $\beta h \gtrsim 1$

Consider now more complicated case $\beta h \ge 1$.

Proposition 28.2.9. *Let $\beta h \ge 1$. Then the following estimates hold with $\mu = \|\partial A'\|_\infty$:*

$$|e(x,y,\tau)| \le C\bigl(\beta+\mu\bigr)\bigl(1+\mu^{\frac{1}{2}}h^{\frac{1}{2}}\bigr)h^{-2} \tag{28.2.44}$$

and

$$|((hD-A)_x\cdot\boldsymbol{\sigma})e(x,y,\tau)| \le C\bigl(\beta+\mu\bigr)\bigl(1+\mu^{\frac{1}{2}}h^{\frac{1}{2}}\bigr)h^{-2} \tag{28.2.45}$$

Proof. Without any loss of the generality one can assume that $\mu \le \beta$; otherwise we simply replace β by μ. Consider $(\beta^{-\frac{1}{2}}h^{\frac{1}{2}}, \beta^{-\frac{1}{2}}h^{\frac{1}{2}}, (\mu+1)^{-\frac{1}{2}}h^{\frac{1}{2}})$-box in $\mathbb{R}^3_x$, where recall that $\nabla\times A^0$ is directed along x_3. Without any loss of the generality one can assume that $A^0(z) = A'(z) = 0$ in its center z.

Since both operators $E(\tau)$ and $((hD-A)_x\cdot\boldsymbol{\sigma})E(\tau)$ have their operator norms bounded by c in $\mathscr{L}^2$, one can prove easily that both operators $\phi D^\alpha E(\tau)$ and $\phi D^\alpha((hD-A)_x\cdot\boldsymbol{\sigma})E(\tau)$ have their operator norms bounded by $C\zeta^\alpha$ with $\zeta_1=\zeta_2=\beta^{\frac{1}{2}}h^{-\frac{1}{2}}$ and $\zeta_3=(h^{-1}+\mu^{\frac{1}{2}}h^{-\frac{1}{2}})$ for $\alpha\in\{0,1\}^3$ and ϕ, supported in the mentioned cube.

Then operator norms of both operators $\gamma_x E(\tau)$ and $\gamma_x((hD-A)_x\cdot\boldsymbol{\sigma})E(\tau)$ from $\mathscr{L}^2$ to $\mathbb{C}^q$ do not exceed $C_0\zeta_1\zeta_3^{\frac{1}{2}}$ and therefore the same is true for adjoint operators; recall that γ_z is operator of restriction to $x=z$.

Since $E(\tau)^*=E(\tau)^2=E(\tau)$ we conclude that the left-hand expressions in (28.2.44) and (28.2.45) do not exceed $C\zeta_1^2\zeta_3$ which is exactly the right-hand expressions in both of them. $\square$

Then from equation (27.2.14), which remains valid (see Remark 28.2.4(iii)), we conclude that

$$\|\Delta A'\|_{\mathscr{L}^\infty}\le C\kappa\bigl(\beta+\mu\bigr)\bigl(1+\mu^{\frac{1}{2}}h^{\frac{1}{2}}\bigr) \tag{28.2.46}$$

and therefore

$$\|\partial^2 A'\|_{\mathscr{L}^\infty}\le C\kappa|\log\beta|\bigl(\beta+\mu\bigr)\bigl(1+\mu^{\frac{1}{2}}h^{\frac{1}{2}}\bigr). \tag{28.2.47}$$

Let (28.2.27)) be fulfilled. Then combining (28.2.47) with (28.2.29) and $\|\partial A'\|_{\mathscr{L}^\infty}\le\|\partial^2 A'\|_{\mathscr{L}^\infty}^{\frac{3}{5}}\cdot\|\partial A'\|^{\frac{2}{5}}$ we conclude that

$$\mu\le C\bigl(\kappa|\log\beta|\bigr)^{\frac{3}{5}}\bigl(\beta+\mu\bigr)^{\frac{3}{5}}\bigl(1+h^{\frac{1}{2}}\mu^{\frac{1}{2}}\bigr)^{\frac{3}{5}}\times\kappa^{\frac{1}{5}}\beta^{\frac{1}{5}}$$

and then <u>either</u>

$$1\le\mu h\le C\bigl(\kappa\beta h|\log\beta|\bigr)^{\frac{6}{7}}\bigl(\kappa\beta h^2\bigr)^{\frac{2}{7}} \tag{28.2.48}$$

<u>or</u> $\mu h\le 1$. In the former case of (28.2.48)

$$\|\partial A'\|_{\mathscr{L}^\infty}\le C\bigl(\kappa\beta|\log\beta|\bigr)^{\frac{8}{7}}h^{\frac{3}{7}} \tag{28.2.49}$$

and

$$\|\partial^2 A'\|_{\mathscr{L}^\infty}\le C\bigl(\kappa\beta|\log\beta|\bigr)^{\frac{11}{7}}h^{\frac{5}{7}}. \tag{28.2.50}$$

Observe that the right-hand expression of (28.2.49) is less than $C\beta$ under assumption

$$\kappa\beta h^2|\log\beta|^K\le c \tag{28.2.27*}$$

with sufficiently large K; however the right-hand expression of (28.2.50) is not necessarily less than $C\beta$ under this assumption and we need more delicate arguments.

Without any loss of the generality we can assume that $\partial_3 A_3(z)=0$ (we can reach it by a gauge transformation).

Then considering $(\beta^{-\frac{1}{2}}h^{\frac{1}{2}},\beta^{-\frac{1}{2}}h^{\frac{1}{2}},\nu^{-\frac{1}{3}}h^{\frac{1}{3}})$-box in $\mathbb{R}^3$ we can replace factor $(1+\mu^{\frac{1}{2}}h^{\frac{1}{2}})h^{-1}$ by $(1+\nu^{\frac{1}{3}}h^{\frac{2}{3}})h^{-1}$ in all above estimates with $\nu=\|\partial^2 A'\|_{\mathscr{L}^\infty}$ and therefore (28.2.47) is replaced by

$$\nu \le C\kappa|\log\beta|\beta\bigl(1+\nu^{\frac{1}{3}}h^{\frac{2}{3}}\bigr)$$

and then under assumption $(28.2.27)^*$

$$\nu=\|\partial^2 A'\|_{\mathscr{L}^\infty}\le C\kappa|\log\beta|\beta \tag{28.2.51}$$

which implies

$$\|\partial A'\|_{\mathscr{L}^\infty}\le C(\kappa|\log\beta|\beta)^{\frac{4}{5}}. \tag{28.2.52}$$

Obviously, if $\mu h\le 1$ we arrive to the same conclusion in easier way. Thus we have proven

Proposition 28.2.10. *Let $\beta h\ge 1$, $\kappa\le\kappa^*$ and $(28.2.27)^*$ be fulfilled. Then estimates (28.2.51)–(28.2.52) hold.*

28.3 Microlocal Analysis Unleashed: $\beta h \lesssim 1$

28.3.1 Rough Estimate to a Minimizer

Recall equation (27.2.14) to a minimizer A of $\mathsf{E}(A)$:

$$\frac{2}{\kappa h^2}\Delta A_j(x)=\Phi_j(x):= \\ -\operatorname{Re}\operatorname{tr}\Bigl[\upsigma_j\Bigl(\bigl((hD-A)_x\cdot\boldsymbol{\sigma} e(x,y,\tau)+e(x,y,\tau)\,{}^t(hD-A)_y\cdot\boldsymbol{\sigma}\bigr)\Bigr)\Bigr]|_{y=x}, \tag{27.2.14}$$

where $e(x,y,\tau)$ is the Schwartz kernel of the spectral projector $\uptheta(\tau-H_{A,V})$. In the current framework this equation should be replaced by

$$\frac{2}{\kappa h^2}\Delta\bigl(A_j(x)-A^0_j(x)\bigr)=\Phi_j(x) \tag{28.3.1}$$

with $\Phi_j(x)$ defined above but since $\Delta A^0_j=0$ these two equations are equivalent. We assume in this section that $\beta h\lesssim 1$.

Proposition 28.3.1. *Let* $\beta h \lesssim 1$ *and let*

$$\|\partial A'\|_{\mathscr{L}^\infty} \le \mu \le h^{-1}. \tag{28.3.2}$$

Then for $\theta \in [1,2]$

$$\|\Phi_j\|_{\mathscr{L}^\infty} + \|h\partial\Phi_j\|_{\mathscr{L}^\infty} \le Ch^{-2}\Bigl(1 + \beta^{\frac{3}{2}} h^{\frac{1}{2}} + |\log h| + (\beta h)^{\frac{\theta-1}{\theta+1}}\|\partial A'\|_{\mathscr{C}^\theta}^{\frac{1}{\theta+1}} + (\beta h)^{\frac{\theta-1}{\theta+1}}\|\partial V\|_{\mathscr{C}^\theta}^{\frac{1}{\theta+1}}\Bigr). \tag{28.3.3}$$

Proof. (i) Assume first that $V \asymp 1$,

$$\beta h^{\frac{1}{3}} \lesssim 1 \qquad \text{and} \qquad \mu = 1. \tag{28.3.4}$$

Note that we need to consider only case $\beta \ge 2$ because otherwise estimate has been proven in Section 27.2 (see Proposition 27.2.16). Then the contribution of the zone $\mathcal{Z}'_\rho \coloneqq \{|\xi_3 - A_3(x)| \le \rho\}$ with $\rho \ge \rho_* \coloneqq C_0\beta^{-1}$ to the Tauberian remainder with $T = T_* \coloneqq \epsilon\beta^{-1}$ does not exceed

$$Ch^{-2}\rho\Bigl(\beta + h^{\frac{1}{2}(\theta-1)}\|\partial A'\|_{\mathscr{C}^\theta}^{\frac{1}{2}} + h^{\frac{1}{2}(\theta-1)}\|\partial V\|_{\mathscr{C}^\theta}^{\frac{1}{2}}\Bigr). \tag{28.3.5}$$

Indeed, if Q is h-pseudodifferential operator supported in this zone then exactly as in the proof of (27.2.48) for $T \le T_*$

$$|F_{t\to h^{-1}\tau}\bar\chi_T(t)\Gamma_x\bigl((hD)^k Q_x U_\varepsilon\bigr)| \le C\rho h^{-2}$$

and

$$|F_{t\to h^{-1}\tau}\bar\chi_T(t)\Gamma_x\bigl((hD)^k Q_x (U - U_\varepsilon)\bigr)| \le C\rho h^{-4}\vartheta T^2,$$

where U and U_ε are Schwartz kernels of $e^{-ih^{-1}tH_{A,V}}$ and $e^{-ih^{-1}tH_{A_\varepsilon,V_\varepsilon}}$ respectively and ϑ is an operator norm of perturbation $\bigl(H_{A_\varepsilon,V_\varepsilon} - H_{A,V}\bigr)$, A_ε and V_ε are ε-mollification of A and V respectively and $\varepsilon \ge h$; then

$$|F_{t\to h^{-1}\tau}\bar\chi_T(t)\Gamma_x\bigl((hD)^k Q_x U\bigr)| \le C\rho(h^{-2} + h^{-4}\vartheta T^2)$$

and therefore the Tauberian error does not exceed $C\rho(h^{-2}T^{-1} + h^{-4}\vartheta T)$.

Optimizing by $T \le T_*$ we get $C\rho\bigl(h^{-2}\rho^{-1} + h^{-3}\vartheta^{\frac{1}{2}}\bigr)$ with $\varepsilon = h$ and $\vartheta = \varepsilon^{\theta+1}\|\partial A'\|_{\mathscr{C}^\vartheta}$, which is exactly the (28.3.5).

Further, following arguments of Section 27.2 we conclude that an error when we pass from the Tauberian expression to the Weyl expression does not exceed

$$C\rho h^{-2}\Bigl(1 + h^{\frac{1}{2}(\theta-1)}\|\partial A'\|_{\mathscr{C}^\theta}^{\frac{1}{2}} + h^{\frac{1}{2}(\theta-1)}\|\partial V\|_{\mathscr{C}^\theta}^{\frac{1}{2}}\Bigr). \tag{28.3.6}$$

(ii) On the other hand, the contribution of zone $\mathcal{Z}_\rho = \{|\xi_3 - A_3(x)| \asymp \rho\}$ with $\rho \ge \rho_* = C_0\beta^{-1}$ to the Tauberian remainder with $T = T^* := \epsilon\rho$ does not exceed

$$Ch^{-2}\Bigl(1 + \rho^{\frac{1}{2}(1-\theta)}h^{\frac{1}{2}(\theta-1)}\|\partial A'\|^{\frac{1}{2}}_{\mathscr{C}^\theta} + \rho^{\frac{1}{2}(1-\theta)}h^{\frac{1}{2}(\theta-1)}\|\partial V\|^{\frac{1}{2}}_{\mathscr{C}^\theta}\Bigr). \tag{28.3.7}$$

Indeed, if Q is h-pseudodifferential operator, supported in this zone, then for $T \le T^*$

$$|F_{t\to h^{-1}\tau}\bar{\chi}_T(t)\Gamma_x\bigl((hD)^k Q_x U_\varepsilon\bigr)| \le C\rho h^{-2},$$

and for $T_* \le T \le T^*$

$$|F_{t\to h^{-1}\tau}\chi_T(t)\Gamma_x\bigl((hD)^k Q_x U_\varepsilon\bigr)| \le C\rho h^{-2}(h/T\rho^2)^s,$$

and then

$$|F_{t\to h^{-1}\tau}\bigl(\bar{\chi}_T(t) - \bar{\chi}_{T_*}(t)\bigr)\Gamma_x\bigl((hD)^k Q_x U_\varepsilon\bigr)| \le C\rho h^{-2}(\beta h/\rho^2)^s$$

and

$$|F_{t\to h^{-1}\tau}\bar{\chi}_T(t)\Gamma_x\bigl((hD)^k Q_x U_\varepsilon\bigr)| \le C\rho h^{-2},$$

while approximation error is estimated in the same way as before but with $\varepsilon = h\rho^{-1}$ and thus ϑ acquires factor $\rho^{-1-\theta}$.

Then the Tauberian error is estimated and optimized by $T \le T^*$ and it does not exceed (28.3.7).

Following arguments of Section 27.2 we conclude that an error when we pass from the Tauberian expression to the Weyl expression does not exceed (28.3.6).

Then the summation of the Tauberian error with respect to ρ ranging from $\rho = \rho'$ to $\rho = 1$ (where in what follows we use ρ instead of ρ' notation) returns

$$Ch^{-2}\Bigl(1 + |\log\rho| + \rho^{-\frac{1}{2}(\theta-1)}h^{\frac{1}{2}(\theta-1)}\|\partial A'\|^{\frac{1}{2}}_{\mathscr{C}^\theta} + \rho^{-\frac{1}{2}(\theta-1)}h^{\frac{1}{2}(\theta-1)}\|\partial V\|^{\frac{1}{2}}_{\mathscr{C}^\theta}\Bigr) \tag{28.3.8}$$

and adding contribution of zone $\mathcal{Z}'_\rho$ we conclude that the total Tauberian remainder does not exceed

$$Ch^{-2}\Bigl(\beta\rho + |\log\rho| + \rho^{-\frac{1}{2}(\theta-1)}h^{\frac{1}{2}(\theta-1)}\|\partial A'\|^{\frac{1}{2}}_{\mathscr{C}^\theta} + \rho^{-\frac{1}{2}(\theta-1)}h^{\frac{1}{2}(\theta-1)}\|\partial V\|^{\frac{1}{2}}_{\mathscr{C}^\theta}\Bigr). \tag{28.3.9}$$

Meanwhile, the summation of the Tauberian-to-Weyl error with respect to ρ returns (28.3.9) albeit without logarithmic term. Optimizing with respect to $\rho \ge \rho_*$ we arrive to

$$Ch^{-2}\Bigl(1 + |\log h| + (\beta h)^{\frac{\theta-1}{\theta+1}} \|\partial A'\|_{\mathscr{C}^\theta}^{\frac{1}{\theta+1}} + (\beta h)^{\frac{\theta-1}{\theta+1}} \|\partial V\|_{\mathscr{C}^\theta}^{\frac{1}{\theta+1}}\Bigr). \tag{28.3.10}$$

Furthermore, observe that

(28.3.11) If in ϵ-vicinity of x inequality $|\nabla V| \le \zeta$ holds (with $\zeta \ge |\log h|^{-1}$), then we can pick up $T^* = \epsilon \min(\zeta^{-1}\rho, 1)$.

Indeed, we can introduce

$$p'_3 := \xi_3 - A_3 - \beta^{-1}\alpha_1(\xi_1 - A_1) - \beta^{-1}\alpha_2(\xi_2 - A_2)$$

such that $\{H, p'_3\} = V_{\xi_3} + O(\nu\beta^{-1})$ with $\nu := \|\partial^2 A\|_{\mathscr{C}^\infty}$.

Therefore, in this case the remainder does not exceed

$$Ch^{-2}\Bigl(1 + \zeta|\log h| + (\beta h)^{\frac{\theta-1}{\theta+1}} \|\partial A'\|_{\mathscr{C}^\theta}^{\frac{1}{\theta+1}} + (\beta h)^{\frac{\theta-1}{\theta+1}} \|\partial V\|_{\mathscr{C}^\theta}^{\frac{1}{\theta+1}}\Bigr). \tag{28.3.12}$$

(iii) Finally, observe that the Weyl expression for Φ_j is just 0. Therefore under assumption (28.3.4) slightly improved estimate (28.3.3) has been proven: $\|\Phi_j\|_{\mathscr{L}^\infty} + \|h\partial\Phi_j\|_{\mathscr{L}^\infty}$ does not exceed expression (28.3.12).

(iv) To get rid of assumption (28.3.4) we scale $x \mapsto x\gamma^{-1}$, $h \mapsto h\gamma^{-1}$, $\beta \mapsto \beta\gamma$ and pick up $\gamma = \min\bigl((\beta h^{\frac{1}{3}})^{-\frac{3}{2}}, \mu^{-1}\bigr)$; then $\beta h \mapsto \beta h$, and $Ch^{-2} \mapsto Ch^{-2}\gamma^{-1} = C\beta^{\frac{3}{2}}h^{-\frac{3}{2}} + C\mu h^{-2}$ (as we need to multiply by γ^{-3}) and both $\|\partial A'\|_{\mathscr{C}^\theta}^{\frac{1}{\theta+1}}$ and $\|\partial V\|_{\mathscr{C}^\theta}^{\frac{1}{\theta+1}}$ acquire factor γ.

Observing that we can take $\zeta = C\gamma$ and that factor γ also pops up in all other terms (except 1) in (28.3.12) we arrive to estimate (28.3.3).

Furthermore, to get rid of assumption $V \asymp 1$ we also can scale with $\gamma = \epsilon|V| + h^{\frac{2}{3}}$ and multiply operator by γ^{-1}; then $h \mapsto h\gamma^{-\frac{3}{2}}$, $\beta \mapsto \beta\gamma^{\frac{1}{2}}$ and estimate (28.3.3) does not deteriorate; we need to multiply by $\gamma^{\frac{1}{2}}$ which does not hurt. $\square$

Remark 28.3.2. (i) We can use $\theta'\neq\theta$ for norm of V.

(ii) If V is smooth enough we can skip the related term (details later).

(iii) We can take $\theta=1$ but in this case factor $\rho^{-\frac{1}{2}(\theta-1)}h^{\frac{1}{2}(\theta-1)}$ in (28.3.8) (i.e. after summation) and in (28.3.9) is replaced by $|\log\rho|$; then taking into account (i) we replace (28.3.10) by

$$Ch^{-2}\Bigl(1+|\log h|+|\log h|\cdot\|\partial A'\|^{\frac{1}{2}}_{\mathscr{C}^1}+(\beta h)^{\frac{\theta'-1}{\theta'+1}}\|\partial V\|^{\frac{1}{\theta'+1}}_{\mathscr{C}^{\theta'}}\Bigr) \tag{28.3.10$'$}$$

and similarly we deal with (28.3.12) and (28.3.3):

$$\|\Phi_j\|_{\mathscr{L}^\infty}+\|h\partial\Phi_j\|_{\mathscr{L}^\infty}\le\\ Ch^{-2}\Bigl(1+\beta^{\frac{3}{2}}h^{\frac{1}{2}}+|\log h|+|\log h|\|\partial A'\|^{\frac{1}{2}}_{\mathscr{C}^1}+(\beta h)^{\frac{\theta'-1}{\theta'+1}}\|\partial V\|^{\frac{1}{\theta'+1}}_{\mathscr{C}^{\theta'}}\Bigr). \tag{28.3.3$'$}$$

(iv) From the very beginning we could assume that $\mu\le\beta$; otherwise we could rescale as above with $\gamma=\beta^{-1}$ and apply arguments of Section 27.2 simply ignoring external field.

Corollary 28.3.3. *Let in the framework of Proposition 28.3.1 A' be a minimizer. Then for $\theta,\theta'\in[1,2]$*

$$|\log h|^{-1}\|\partial A'\|_{\mathscr{C}^1}+h^{\theta-1}\|\partial A'\|_{\mathscr{C}^\theta}\\ \le C\kappa\Bigl(\beta^{\frac{3}{2}}h^{\frac{1}{2}}+|\log h|+\mu+(\beta h)^{\frac{1}{2}(\theta'-1)}\|V\|^{\frac{1}{2}}_{\mathscr{C}^{\theta'+1}}\Bigr)\\ +C\kappa^2|\log h||\log h|^2+C\|\partial A'\|. \tag{28.3.13}$$

Proof. Indeed, the left-hand expression of (28.3.13) does not exceed

$$\|\Delta A'\|_{\mathscr{L}^\infty}+\|h\partial\Delta A'|_{\mathscr{L}^\infty}+C\|\partial A'\|$$

while for a minimizer $\|\Delta A'\|_{\mathscr{L}^\infty}+\|h\partial\Delta A'|_{\mathscr{L}^\infty}$ does not exceed the right-hand expression of (28.3.3) multiplied by $C\kappa h^2$. □

28.3.2 Microlocal Analysis

As long as $\beta\le C_0h^{-\frac{1}{3}}$ we are rather happy with our result here, but we want to improve it otherwise. First we will prove that singularities propagate along magnetic lines; however since we do not know a self-generated magnetic field we just consider all possible lines which will be in the cone $\{(x,y)\colon |x'-y'|\le C_0\mu\beta^{-1}T\}$ where $1\le\mu\le\beta$.

Proposition 28.3.4. *Assume that* $\beta h \lesssim 1$,

$$\|V\|_{\mathscr{C}^1(B(0,2))} \le C_0 \tag{28.3.14}$$

and

$$\|\partial A'\|_{\mathscr{C}(B(0,2))} \le \mu \qquad (1 \le \mu \le \epsilon\beta) \tag{28.3.15}$$

with sufficiently small constant $\epsilon > 0$.

Let $U(x,y,t)$ *be the Schwartz kernel of* $e^{ih^{-1}tH_{A,V}}$. *Then*

(i) For $T \asymp 1$ *estimate*

$$\|F_{t\to h^{-1}\tau}\bar{\chi}_T(t)\psi_1(x)\psi_2(y)U\| \le Ch^s \tag{28.3.16}$$

holds for all $\psi_1,\psi_2 \in \mathscr{C}_0^\infty(B(0,1))$, *such that* $\operatorname{dist}(\operatorname{supp}(\psi_1),\operatorname{supp}(\psi_2)) \ge C_0T$ *and* $\tau \le c_0$; *here* $\|.\|$ *means an operator norm from* $\mathscr{L}^2$ *to* $\mathscr{L}^2$ *and* s *is arbitrarily large.*

(ii) For $\bar{\rho} \le \rho \lesssim 1$ *with* $\bar{\rho} := C_0\mu\beta^{-1}$ *and* $T \asymp \rho$ *estimate*

$$\begin{multline}\|F_{t\to h^{-1}\tau}\bar{\chi}_T(t)\varphi_1(\rho^{-1}p_{3x})\varphi_2(\rho^{-1}p_{3y})\psi_1(x)\psi_2(y)U\|\\ \le C\rho^{1-3s}h^s + C\rho^{2-\theta}h^\theta\bigl(\|A'\|_{\theta+1} + \|V\|_{\theta+1}\bigr)\end{multline} \tag{28.3.17}$$

holds for all all $\varphi_1,\varphi_2 \in \mathscr{C}_0^\infty$, $\psi_1,\psi_2 \in \mathscr{C}_0^\infty(B(0,1))$, *such that* $\operatorname{dist}(\operatorname{supp}(\varphi_1),\operatorname{supp}(\varphi_2)) \ge C_0$, *and* $\tau \le c_0$; *here and below* $p_j = hD_j - A_j$, $p_j^0 = hD_j - A_j^0$.

(iii) For $\bar{\rho} \le \rho \lesssim 1$ *and* $T \asymp \rho \lesssim 1$ *estimate*

$$\begin{multline}\|F_{t\to h^{-1}\tau}\bar{\chi}_T(t)\varphi_1(\rho^{-1}p_{3x})\varphi_2(\rho^{-1}p_{3y})\psi_1(\gamma^{-1}x)\psi_2(\gamma^{-1}y)U\|\\ \le C\rho^{1-s}\gamma^{-s}h^s + Ch^\theta\gamma\rho^{-\theta}\bigl(\|A'\|_{\theta+1} + \|V\|_{\theta+1}\bigr)\end{multline} \tag{28.3.18}$$

holds for all $\varphi_1,\varphi_2 \in \mathscr{C}_0^\infty$, $\psi_1,\psi_2 \in \mathscr{C}_0^\infty$, *such that* $\operatorname{dist}(\operatorname{supp}(\psi_1),\operatorname{supp}(\psi_2)) \ge C_0$, $\gamma = \rho T \ge \beta^{-1}$, $\rho\gamma \ge h$ *and* $\tau \le c_0$.

Proof. Statement (i) claims that the general propagation speed with respect to x is bounded by C_0. Further, Statement (ii) claims that the on distances $\ge C_0\bar{\rho}$ the propagation speed with respect to p_3 is also bounded by C_0. Finally, Statement (iii) claims that on distances $\ge C_0\bar{\rho}$ the propagation speed with respect to x is bounded by $C_0\rho$. Note that from Corollary 28.3.3 we know that $\mu \lesssim \beta$.

(a) Proof follows the proof of Proposition 27.2.11 in the framework of the strong magnetic field. Namely, proof of Statement (i) is a straightforward repetition of the proof of Proposition 27.2.11(i). Since here we do not apply at this stage operators $(hD_x)^\alpha$ and $(hD_y)^{\alpha'}$, no assumption to the smoothness of A is needed.

(b) Assume that $A_3\equiv 0$ (we will get rid of this assumption on the next step). After Statement (i) has been proven we rescale $t\mapsto t/T$, $x_3\mapsto x_3/\gamma$ with $\gamma=\rho T$ (since φ_l depend only on ξ_3, all other coordinates are rather irrelevant), $h\mapsto \hbar=h/(\rho\gamma)$, $T\mapsto 1$. Then we apply the arguments used in the proof of Proposition 27.2.11(ii) and conclude that the left-hand expression of (28.3.17) does not exceed

$$T\Bigl(\hbar^s + C\hbar^\theta\gamma^{\theta+1}\bigl(\||A'\||_{\theta+1}+\||V\||_{\theta+1}\bigr)\Bigr),$$

where factor T is due to the scaling in the Fourier transform and $\gamma^{\theta+1}$ is due to the scaling in $\||\cdot\||$-norms. Plugging $\hbar$, T, and $\gamma=\rho^2$ we get the right-hand expression of (28.3.17).

Then if ψ_l depend only on x_3, y_3 we can follow the proof of Proposition 27.2.11(iii) and prove Statement (iii).

(c) Let A_3 be not necessarily identically 0. To consider ψ_l depending only on x_1 or x_2 we should introduce (in the standard magnetic Schrödinger manner) $x'_1:=x_1+\beta^{-1}p^0_2$ or $x'_2:=x_2-\beta^{-1}p^0_1$ respectively; recall that $p^0_j=hD_j-A^0_j$ and $p_j=hD_j-A_j$, $j=1,2,3$.

Then $[p^0_1,p^0_2]=ih\beta^{-1}$, $[p^0_j,x_k]=-ih\delta_{jk}$, $[p^0_j,x'_k]=0$ and one can see easily that $[p_j,x'_k]=O(\beta^{-1}\mu h)$ (for any $\mu: 1\le\mu\le\beta$) for $j=1,2,3$ and $k=1,2$. Now we can apply the same arguments as above as long as $\rho\ge\bar\rho$.

(d) Next we need to recover Statement (ii) in the general case. Without any loss of the generality we may consider a vicinity of point z where $A'(z)=0$ and also $\partial A'(z)=0$. Indeed we can achieve the former by the gauge transformation and the latter by a rotation of coordinates in which case increment of p^0_3 will be $O(\bar\rho)$.

In this case we just repeat the same arguments of Part (b) of our proof.

(e) Finally, the proof of Statement (iii) as ψ_l depend only on x_3 follows from Statement (ii).

We leave all easy details to the reader. □

Proposition 28.3.5. *Let* $\beta h \lesssim 1$ *and assumptions* (28.3.14) *and* (28.3.15) *be fulfilled. Then*

(i) For $h \le T \le 1$ *estimate*

$$|F_{t\to h^{-1}\tau}\bar{\chi}_T(t)p_x^\alpha p_y^{\alpha'} U| \le CT^{-s}h^{-3+s} \tag{28.3.19}$$

holds for all $\alpha : |\alpha| \le 2$, $\alpha' : |\alpha'| \le 2$, *and all* $x, y \in B(0,1)$, *such that* $|x-y| \ge C_0 T$ *and* $\tau \le c_0$.

(ii) In the framework of Proposition 28.3.4(ii) the following estimate holds for all $\alpha : |\alpha| \le 2$, $\alpha' : |\alpha'| \le 2$, *and* $\tau \le c$:

$$\begin{aligned} &|F_{t\to h^{-1}\tau}\bar{\chi}_T(t)p_x^\alpha p_y^{\alpha'} \varphi_1(\rho^{-1}p_{3x})\varphi_2(\rho^{-1}p_{3y})\psi_1(x)\psi_2(y)U| \\ &\qquad \le C\rho h^{-1}\bigl(\beta h^{-1}+\rho^2 h^{-2}\bigr)\Bigl(\rho^{1-3s}h^s + \rho^{2-\theta}h^\theta\bigl(\|A'\|_{\theta+1}+\|V\|_{\theta+1}\bigr)\Bigr); \end{aligned} \tag{28.3.20}$$

(iii) In the framework of Proposition 28.3.4(iii) the following estimate holds for all $\alpha : |\alpha| \le 2$, $\alpha' : |\alpha'| \le 2$, *and* $\tau \le c$:

$$\begin{aligned} &|F_{t\to h^{-1}\tau}\bar{\chi}_T(t)p_x^\alpha p_y^{\alpha'} \varphi_1(\rho^{-1}p_{3x})\varphi_2(\rho^{-1}p_{3y})\psi_1(\gamma^{-1}x)\psi_2(\gamma^{-1}y)U| \\ &\qquad \le C\rho h^{-1}\bigl(\beta h^{-1}+\rho^2 h^{-2}\bigr)\Bigl(\rho^{1-s}\gamma^{-s}h^s + h^\theta\gamma\rho^{-\theta}\bigl(\|A'\|_{\theta+1}+\|V\|_{\theta+1}\bigr)\Bigr). \end{aligned} \tag{28.3.21}$$

Proof. Observe that estimates (28.3.16)–(28.3.18) hold if one applies operator $p_x^\alpha p_y^{\alpha'}$ under the norm (this follows from equations for U by (x,t) and dual equations by (y,t)). Then estimates (28.3.19)–(28.3.21) hold with $\alpha = \alpha' = 0$.

Really, without any loss of the generality one can assume that $A' = 0$ at some point of $\mathsf{supp}(\psi_1)$; then estimates (28.3.16)–(28.3.18) hold if one applies operator $p_x^{0\alpha}p_y^{0\alpha'}$ instead. Then estimate (28.3.19) holds with $\alpha = \alpha' = 0$; further, estimates (28.3.20)–(28.3.21) also hold with $\alpha = \alpha' = 0$ if one applies an extra factor $\bar{\varphi}_1(\rho^{-1}p_{3x}^0)\bar{\varphi}_2(\rho^{-1}p_{3y}^0)$ under the norm (this follows from the properties of p_j^0, $j = 1,2,3$, in particular, canonical form). However if $\bar{\varphi}_l = 1$ in ϵ-vicinity of $\mathsf{supp}(\varphi_l)$ then we can skip this factor.

Finally, appealing to equations for U by (x,t) and (y,t) again we recover estimates (28.3.19)–(28.3.21) with $|\alpha| \le 2$, $|\alpha'| \le 2$. □

Proposition 28.3.6. *Let $\beta h \lesssim 1$ and (28.3.14) and (28.3.15) be fulfilled. Let $z \in B(0,1)$. Then:*

(i) The following estimate

$$|F_{t\to h^{-1}\tau}\bar{\chi}_T(t)p_x^\alpha p_y^{\alpha'}\varphi_1(\rho^{-1}p_{3x})\varphi_2(\rho^{-1}p_{3y})U|_{x=y=z}| \\ \le C\rho T h^{-1}\bigl(\beta h^{-1}+\rho^2 h^{-2}\bigr) \tag{28.3.22}$$

holds for all $\alpha : |\alpha|\le 2$, $\alpha' : |\alpha'|\le 2$, and $\tau \le c$.

(ii) Let $A_z(x) = A(z) + \langle x-z, \nabla_z\rangle A(z)$, $V_z(x) = V(z) + \langle x-z,\nabla_z\rangle V(z)$ be linear approximations to A and V at z; let $H_z = H_{A_z,V_z}$, $U_z(x,y,t)$ be its Schwartz kernel. Then for $h^{1-\delta}\le T\le C_0$, $\rho \le C_0$ estimate

$$|F_{t\to h^{-1}\tau}\bar{\chi}_T(t)p_x^\alpha p_y^{\alpha'}\varphi_1(\rho^{-1}p_{3x})\varphi_2(\rho^{-1}p_{3y})(U-U_z)|_{x=y=z}| \\ \le C\rho T^2 h^{-2}\bigl(\beta h^{-1}+\rho^2 h^{-2}\bigr)\nu\gamma^2 \tag{28.3.23}$$

holds with

$$\gamma=\gamma(\rho,T) \coloneqq C_0(\rho+T)T + C_0 h\rho^{-1}, \tag{28.3.24}$$

and

$$\nu = \bigl(\|\!|A'|\!\|_2 + \|\!|V|\!\|_2\bigr)+\mu^2. \tag{28.3.25}$$

Proof. (i) Proof of Statement (i) is easy and left to the reader.

(ii) To prove Statement (ii) observe that

$$e^{ith^{-1}H} = e^{ith^{-1}H_z} + ih^{-1}\int_0^t e^{i(t-t')h^{-1}H}(H-H_z)e^{it'h^{-1}H_z}\,dt' = \\ e^{ith^{-1}H_z} + \sum_{0\le k\le K} \underbrace{ih^{-1}\int_0^t e^{i(t-t')h^{-1}H}(H-H_z)\psi_k e^{it'h^{-1}H_z}\,dt'}, \tag{28.3.26}$$

where ψ_0 is a γ-admissible function supported in $B(z,2\gamma)$ and ψ_k are γ_k-admissible functions supported in $B(z,\gamma_k)\setminus B(z,\frac{1}{2}\gamma_k)$ with $\gamma_k = 2^k\gamma$. Plugging (28.3.26) into the left-hand expression of (28.3.23) we note that the first term is cancelled and we have the sum with respect to $k : 0\le k\le K$ obtained from this expression when we replace $(U-U_z)$ by the Schwartz kernel of the selected above term.

Further, observe that the term with $k=0$ does not exceed the right-hand expression of (28.3.23).

Furthermore, terms with $k : 1\le k\le K$ do not exceed the right-hand expression of (28.3.21) multiplied by $CTh^{-1}\min(\nu\gamma_k^2,1)$; indeed, we just replace ρ by T if needed. After summation with respect to $k: 0\le k\le K$ we get

$$C\rho h^{-1}T\bigl(\beta h^{-1}+\rho^2h^{-2}\bigr)\times\Bigl(\rho^{-s}\gamma^{-s}h^s\min(\nu\gamma^2,1)+h^2\rho^{-2}\nu\min(\nu,1)\Bigr)$$

which again does not exceed the right-hand expression of (28.3.23). □

Remark 28.3.7. Actually Statement (ii) is better than Statement (i) only if $\nu\gamma^2Th^{-1}\le 1$.

28.3.3 Advanced Estimate to a Minimizer

Now we are going to apply the results of the previous Subsection 28.3.2 to the right-hand expression of (27.2.14).

Tauberian Estimate

Consider different zones (based on the magnitude of $|p_3|$). Recall that $\bar\rho=\beta^{-1}$ [5] and $\rho^*=(\beta h)^{\frac12}$.

Zone $\{\rho'\lesssim|p_3|\lesssim\rho^*\}$. Observe that Proposition 28.3.6(ii) implies that for $\varphi_j\in\mathscr{C}_0^\infty([-2,-\frac12]\cup[\frac12,2])$ estimate

$$|F_{t\to h^{-1}\tau}\bar\chi_T(t)p_x^\alpha p_y^{\alpha'}\varphi_1(\rho^{-1}p_{3x})\varphi_2(\rho^{-1}p_{3y})U|_{x=y=z}|\le CS(\rho,T) \tag{28.3.27}$$

holds with

$$S(\rho,T)=\bigl(\beta h^{-1}+\rho^2h^{-2}\bigr)\bigl(\rho^{-1}+\rho h^{-2}\nu\gamma^2T^2\bigr), \tag{28.3.28}$$

where $\gamma=\gamma(\rho,T)$ is defined by (28.3.24).

Indeed, one can prove easily that

$$|F_{t\to h^{-1}\tau}\bar\chi_T(t)p_x^\alpha p_y^{\alpha'}\varphi_1(\rho^{-1}p_{3x})\varphi_2(\rho^{-1}p_{3y})U_z|_{x=y=z}|\\ \le C(\beta h^{-1}\rho^{-1}+\rho^2h^{-2}). \tag{28.3.29}$$

[5] As we assume that $\mu=1$; otherwise $\bar\rho=\mu\beta^{-1}$.

Let us take $\alpha=\alpha'$, $\varphi_1=\varphi_2$ and $\rho_1=\rho_2$. Since in this case expression

$$p_x^\alpha p_y^{\alpha'}\varphi_1(\rho_1^{-1}p_{3x})\varphi_2(\rho_2^{-1}p_{3y})e(.,.,\tau)|_{x=y} \tag{28.3.30}$$

is a monotone function with respect to τ, then the standard Tauberian arguments (part I–estimates; we leave easy details to the reader) imply that

$$\begin{gathered}|p_x^\alpha p_y^\alpha\varphi_1(\rho^{-1}p_{3x})\varphi_1(\rho^{-1}p_{3y})\bigl[e(.,.,\tau)-e(.,.,\tau')\bigr]|_{x=y}|\\ \le CS(\rho,T)\bigl(T^{-1}+|\tau-\tau'|h^{-1}\bigr)\end{gathered} \tag{28.3.31}$$

for all $\tau'\le\tau\le c$ and therefore

$$\begin{gathered}|p_x^\alpha p_y^{\alpha'}\varphi_1(\rho_1^{-1}p_{3x})\varphi_2(\rho_2^{-1}p_{3y})\bigl[e(.,.,\tau)-e(.,.,\tau')\bigr]|_{x=y}|\\ \le C\bigl(S(\rho_1,T_1)S(\rho_2,T_2)\bigr)^{\frac12}\Bigl(T_1^{-\frac12}T_2^{-\frac12}+|\tau-\tau'|^{\frac12}\bigl(T_1^{-\frac12}+T_2^{-\frac12}\bigr)h^{-\frac12}+|\tau-\tau'|h^{-1}\Bigr).\end{gathered} \tag{28.3.32}$$

Then the standard Tauberian arguments (part II–asymptotics, with the minor modifications; again we leave easy details to the reader) imply that expression (28.3.30) is given by the standard Tauberian formula with an error, not exceeding the right-hand expression of (28.3.32) with $|\tau-\tau'|$ replaced by hT^{-1}, which is

$$C\bigl(S(\rho_1,T_1)S(\rho_2,T_2)\bigr)^{\frac12}\Bigl(T_1^{-\frac12}T_2^{-\frac12}+\bigl(T_1^{-\frac12}+T_2^{-\frac12}\bigr)T^{-\frac12}+T^{-1}\Bigr). \tag{28.3.33}$$

Note that for $T\ge\max(T_1,T_2)$ the second factor in (28.3.33) is $\asymp T_1^{-\frac12}T_2^{-\frac12}$.

In other words, a contribution of the pair (ρ_1,ρ_2) to the Tauberian error does not exceed a square root of $S(\rho_1,T_1)T_1^{-1}\times S(\rho_2,T_2)T_2^{-1}$ with

$$\begin{gathered}S(\rho,T)T^{-1}=\beta h^{-1}\Bigl(\rho^{-1}T^{-1}+h^{-2}\rho\nu T\bigl(T^4+\rho^2T^2+h^2\rho^{-2}\bigr)\Bigr)\\ \asymp\beta h^{-1}\Bigl(\rho^{-1}T^{-1}+h^{-2}\nu\rho^3T^3+h^{-2}\nu\rho T^5+\nu\rho^{-1}T\Bigr)\\ \text{for}\quad\bar\rho\le\rho\le\rho^*.\end{gathered} \tag{28.3.34}$$

Minimizing this expression by $h\le T\lesssim 1$ we get

$$\begin{gathered}\beta h^{-1}\Bigl(\rho^{-\frac34}(h^{-2}\nu\rho^3)^{\frac14}+\rho^{-\frac56}(h^{-2}\nu\rho)^{\frac16}+\rho^{-1}\nu^{\frac12}\Bigr)\\ \asymp\beta h^{-1}\Bigl(h^{-\frac12}\nu^{\frac14}+h^{-\frac13}\nu^{\frac16}\rho^{-\frac23}+\nu^{\frac12}\rho^{-1}\Bigr);\end{gathered}$$

then the summation by $\rho\in[\rho',\rho^*]$ returns

$$\beta h^{-1}\Bigl(h^{-\frac{1}{2}}\nu^{\frac{1}{4}}|\log h| + h^{-\frac{1}{3}}\nu^{\frac{1}{6}}\rho^{-\frac{2}{3}} + \nu^{\frac{1}{2}}\rho^{-1}\Bigr) \tag{28.3.35}$$

with $\rho=\rho'$ to be selected later.

Zone $\{\rho^*\lesssim |p_3|\lesssim 1\}$. Further, we claim that

(28.3.36) For $h^{\frac{1}{3}}\le\rho\le C_0$, $h\le T\le \epsilon_0\rho$ we can take $\gamma=h\rho^{-1}$.

Indeed, observe that if we use ε-approximation with $\varepsilon=(\rho^{-1}h)^{1-\delta}$ then the contribution of time intervals $\{t\colon T_*\le |t|\le T^*\}$ with $T_*=\rho^{-1}(\rho^{-1}h)^{1-\delta}$, $T^*=\epsilon_0\rho$ is negligible and the transition from $\varepsilon=(\rho^{-1}h)^{1-\delta}$ to $\varepsilon=(\rho^{-1}h)$ is done like in the previous Chapter 26. Again we leave easy details to the reader.

Then

$$S(\rho,T)T^{-1}\asymp \rho h^{-2}\bigl(T^{-1}+\nu T\bigr); \tag{28.3.37}$$

minimizing by $T\colon h\le T\le\epsilon\rho$ we get

$$\rho h^{-2}\bigl(\nu^{\frac{1}{2}}+\rho^{-1}+\nu h\bigr);$$

then summation by $\rho\in[\rho^*,C_0]$ returns

$$h^{-2}\bigl(\nu^{\frac{1}{2}}+(1+\nu h)|\log h|\bigr). \tag{28.3.38}$$

Observe that $\rho^*=(\beta h)^{\frac{1}{2}}\ge h^{\frac{1}{3}}$ as $\beta\ge h^{-\frac{1}{3}}$.

Zone $\{|p_3|\lesssim\rho'\}$. Finally, the remaining zone $\{|p_3|\lesssim\rho'\}$ is covered by a single element $\varphi(\rho^{-1}p_3)$ with $\varphi\in\mathscr{C}_0^\infty([-2,2])$, $\rho=\rho'$.

Then instead of minimized $S(\rho,T)T^{-1}$ we can take $\rho\beta h^{-2}$ which should be added to the sum of expressions (28.3.38) and (28.3.35) which estimate contributions of two other zones resulting in

$$\begin{multline}h^{-2}\bigl(\nu^{\frac{1}{2}}+(1+\nu h)|\log h|\bigr)\\ +\beta h^{-1}\Bigl[h^{-\frac{1}{2}}\nu^{\frac{1}{4}}|\log h| + \underbracket{h^{-\frac{1}{3}}\nu^{\frac{1}{6}}\rho^{-\frac{2}{3}}+\nu^{\frac{1}{2}}\rho^{-1}+\rho h^{-1}}\Bigr].\end{multline} \tag{28.3.39}$$

Obviously the second term in (28.3.39) should be minimized by $\rho=\rho'\in[\bar\rho,\rho^*]$, resulting in

$$\beta h^{-1}\Bigl[h^{-\frac12}\nu^{\frac14}|\log h| + h^{-\frac25}(h^{-\frac13}\nu^{\frac16})^{\frac35} + h^{-\frac12}(\nu^{\frac12})^{\frac12}\Bigr]\\ \asymp \beta h^{-1}\Bigl[h^{-\frac12}\nu^{\frac14}|\log h| + h^{-\frac35}\nu^{\frac1{10}} + h^{-\frac12}\nu^{\frac14})\Bigr];$$

two terms arising when we set $\rho=\rho^*$ in the terms with negative power of ρ and one term arising when we set $\rho=\bar\rho$ in the term with positive power of ρ are absorbed by other terms in (28.3.39), which becomes

$$h^{-2}\bigl(\nu^{\frac12}+(1+\nu h)|\log h|\bigr)\\ +\beta h^{-1}\Bigl[h^{-\frac12}\nu^{\frac14}|\log h| + h^{-\frac35}\nu^{\frac1{10}} + h^{-\frac12}\nu^{\frac14}\Bigr]. \tag{28.3.40}$$

This is an estimate for the whole Tauberian error (with variable $T=T(\rho)$).

Calculating Tauberian Expression

Now we need to consider the Tauberian expression for $p_x^\alpha p_y^{\alpha'}e(.,.,0)|_{x=y=z}$ and estimate an error made when we replace it by the Tauberian expression for $p_x^\alpha p_y^{\alpha'}e_z(.,.,0)|_{x=y=z}$; we will call it the *second error* in contrast to the first (Tauberian) error. Note that we are interested only in the case $|\alpha|+|\alpha'|=1$.

Let us again consider contribution of pair (ρ_1,ρ_2). First, observe that for $\rho_1\asymp\rho_2$ this error does not exceed $CS(\rho_2,T)T^{-1}$ due to our standard arguments and therefore we get for such pairs the same contribution to the total error as we already got for the Tauberian error.

Second, consider pairs with $\rho_1\gg\rho_2$ and in this case redoing previous arguments we observe that the contribution to the first error does not exceed $CS(\rho_1,T)^{\frac12}S(\rho_2,T)^{\frac12}T^{-1}$ and the contribution to the second error does not exceed

$$C\beta h^{-1}\times \rho_1^{\frac12}\rho_2^{\frac12}h^{-2}\nu T^3(T+\rho_2)^2, \tag{28.3.41}$$

where the first term which was $C\beta h^{-1}\rho^{-1}T^{-1}$ in the former case $\rho_1\asymp\rho_2$ simply disappear. Indeed, it appears only due to the contribution of the time interval $\{|t|\le\rho\}$ where we should take $\rho=\max(\rho_1,\rho_2)=\rho_1$ and estimate an error due to the propagation of singularities.

Similarly, the second term leading to expression (28.3.41) would also disappear unless $\rho_1 \lesssim T$ again due to the propagation of singularities. Therefore the combined contribution of any pair to both errors does not exceed

$$\begin{aligned}(28.3.42)\quad &\Bigl(\rho_1^{-1}T^{-1}+\rho_1^3h^{-2}\nu T^3+\rho_1h^{-2}\nu T^5+\rho_1^{-1}\nu T\Bigr)^{\frac{1}{2}}\\ &\times\Bigl(\rho_2^{-1}T^{-1}+\rho_2^3h^{-2}\nu T^3+\rho_2h^{-2}\nu T^5+\rho_2^{-1}\nu T\Bigr)^{\frac{1}{2}}+\rho_1^{\frac{1}{2}}\rho_2^{\frac{1}{2}}h^{-2}\nu T^5,\end{aligned}$$

multiplied by $C\beta h^{-1}$ since we consider at this moment the case of $\rho'\le\rho_2\ll\rho_1\le\rho^*$ while all other cases (namely, $\rho_2\le\rho'\le\rho_1\le\rho^*$; $\rho_2\le\rho'\le\rho^*\le\rho_1$; $\rho'\le\rho_2\le\rho^*\le\rho_1$; and $\rho^*\le\rho_2\ll\rho_1$) are easier and left to the reader.

Opening parenthesis in (28.3.42) and eliminating all smaller terms we arrive to

$$\begin{aligned}&\rho_1^{-\frac{1}{2}}\rho_2^{-\frac{1}{2}}T^{-1}+\rho_1^{\frac{1}{2}}\rho_2^{\frac{1}{2}}h^{-2}\nu T^5+\rho_1^{\frac{3}{2}}\rho_2^{\frac{1}{2}}h^{-2}\nu T^4\\ &+\bigl(\rho_1^{\frac{3}{2}}\rho_2^{\frac{3}{2}}h^{-2}\nu+\rho_1^{\frac{1}{2}}\rho_2^{-\frac{1}{2}}h^{-1}\nu\bigr)T^3+\bigl(\rho_1^{\frac{1}{2}}\rho_2^{-\frac{1}{2}}(h^{-2}\nu)^{\frac{1}{2}}+\rho_1^{\frac{3}{2}}\rho_2^{-\frac{1}{2}}h^{-1}\nu\bigr)T^2\\ &+\bigl(\rho_1^{-\frac{1}{2}}\rho_2^{-\frac{1}{2}}\nu+\rho_1^{\frac{3}{2}}\rho_2^{-\frac{1}{2}}(h^{-2}\nu)^{\frac{1}{2}}\bigr)T+\rho_1^{-\frac{1}{2}}\rho_2^{-\frac{1}{2}}\nu^{\frac{1}{2}};\end{aligned}$$

minimizing by T we get

$$\begin{aligned}&\rho_1^{-\frac{1}{3}}\rho_2^{-\frac{1}{3}}(h^{-2}\nu)^{\frac{1}{6}}+\rho_1^{-\frac{1}{10}}\rho_2^{-\frac{3}{10}}(h^{-2}\nu)^{\frac{1}{5}}+(h^{-2}\nu)^{\frac{1}{4}}+\rho_1^{-\frac{1}{4}}\rho_2^{-\frac{1}{2}}(h^{-1}\nu)^{\frac{1}{4}}\\ &+\rho_1^{-\frac{1}{6}}\rho_2^{-\frac{1}{2}}(h^{-1}\nu)^{\frac{1}{6}}+\rho_1^{-\frac{1}{2}}\rho_2^{-\frac{1}{2}}\nu^{\frac{1}{2}}+\rho_1^{\frac{1}{2}}\rho_2^{-\frac{1}{2}}(h^{-2}\nu)^{\frac{1}{4}}+\underbracket{\rho_1^{-\frac{1}{2}}\rho_2^{-\frac{1}{2}}\nu^{\frac{1}{2}}}.\end{aligned}$$

Observe, that only the last term has ρ_1 in the positive degree. Also observe, that the optimal $T=T(\rho)$ in the Tauberian error is a decreasing function of ρ, so $T_1\le T_2$ where $T_j:=T(\rho_j)$; therefore we consider the Tauberian expression for $T\le T_2$ and thus for $\rho_1\le T\lesssim T_2$.

Therefore T_2 must be an upper bound for ρ_1 and therefore the summation by $\rho_1:\rho_2\le\rho_1\le T_2$ results in all the terms with negative power of ρ_1 in the value as $\rho_1=\rho_2$ and in the exceptional (last) term with $\rho_1=T_2$:

$$\begin{aligned}(28.3.43)\quad &\rho_2^{-\frac{2}{3}}(h^{-2}\nu)^{\frac{1}{6}}+\rho_2^{-\frac{2}{5}}(h^{-2}\nu)^{\frac{1}{5}}+(h^{-2}\nu)^{\frac{1}{4}}|\log\rho_2(\rho_2^{-2}h^2\nu^{-1})^{-\frac{1}{6}}|\\ &+\rho_2^{-\frac{3}{4}}(h^{-1}\nu)^{\frac{1}{4}}+\rho_2^{-1}\nu^{\frac{1}{2}}+(\rho_2^{-2}h^2\nu^{-1})^{\frac{1}{12}}\rho_2^{-\frac{1}{2}}(h^{-2}\nu)^{\frac{1}{4}}\end{aligned}$$

(where we used inequality $T_2 \le (\rho_2^{-2}h^2\nu^{-1})^{\frac{1}{6}}$) with the last term equal to the first one.

Then the summation by $\rho_2 \ge \rho'$ results in the same expression (28.3.43) calculated for $\rho_2 = \rho'$; adding as usual $\rho' h^{-1}$ (asince $\rho'\beta h^{-2}$ estimates the contribution of zone $\{\rho_2 \le \rho'\}$) and minimizing by $\rho' \ge \bar\rho$, we get, after we multiply by βh^{-1} and add contributions of all other zones and also Tauberian estimate (28.3.40), the following expression:

$$h^{-2}\bigl(\nu^{\frac{1}{2}} + (\mu+\nu h)|\log h|\bigr) + \beta h^{-1}\Bigl[h^{-\frac{1}{2}}\nu^{\frac{1}{4}}|\log h| + h^{-\frac{3}{5}}\nu^{\frac{1}{10}} + h^{-\frac{4}{7}}\nu^{\frac{1}{7}} + h^{-\frac{1}{2}}\nu^{\frac{1}{4}}\Bigr]. \tag{28.3.44}$$

Recall that we derived estimate for the difference between $p_x^\alpha p_y^{\alpha'} e(.,.,0)|_{x=y=z}$ and $p_x^\alpha p_y^{\alpha'} e_z(.,.,0)|_{x=y=z}$ and thus for $\mu=1$ we arrive to Statement (i) of Proposition 28.3.8 below for $\mu = 1$.

Observe, however, that in virtue of Subsection 28.3.1 the same estimate holds for $\beta \le h^{-\frac{1}{3}}$. Then, if $1 \le \mu \le \beta$, one can scale $x \mapsto \mu x$, $h \mapsto \mu h$, $\nu \mapsto \mu^2\nu$, $\kappa \mapsto \mu\kappa$ and we arrive to the same statement without assumption $\mu = 1$.

Furthermore, in virtue of Propositions 28.A.4 and 28.A.5, expression $|p_x^\alpha p_y^{\alpha'} e_z(.,.,0)|_{x=y=z}|$ does not exceed $C\beta^{\frac{1}{2}}h^{-2}\|\partial V\|_{\mathscr{L}^\infty}$ if $|\alpha|+|\alpha'| = 1$[6]. Therefore we arrive to Statement (ii) below:

Proposition 28.3.8. *Let $\beta \le h^{-1}$ and* (28.3.14) *and* (28.3.15) *be fulfilled. Then*

(i) $|p_x^\alpha p_y^{\alpha'}\bigl[e(.,.,0) - e_z(.,.,0)\bigr]|_{x=y=z}|$ *does not exceed expression* (28.3.44) *for $|\alpha| \le 2$, $|\alpha'| \le 2$.*

(ii) Consider $|\alpha|+|\alpha'| = 1$; then $|p_x^\alpha p_y^{\alpha'} e(.,.,0)|_{x=y=z}|$ does not exceed expression (28.3.44) *plus $C\omega h^{-2}$ with*

$$\omega = \begin{cases} 1 & \text{if } \beta \le h^{-\frac{1}{3}},\\ \beta^{\frac{3}{2}}h^{\frac{1}{2}} & \text{if } h^{-\frac{1}{3}} \le \beta \le h^{-\frac{1}{2}},\\ \beta^{\frac{1}{2}} & \text{if } h^{-\frac{1}{2}} \le \beta \le h^{-1}. \end{cases} \tag{28.3.45}$$

[6] Actually Proposition 28.A.4 provides better estimate for $\|\partial V\|_{\mathscr{L}^\infty} \le \beta^2 h$.

Remark 28.3.9. (i) Observe that for $\beta \le h^{-\frac{1}{2}}$ we got no improvement over results of Subsection 28.3.1.

(ii) One can replace μ in the definition of $\bar{\rho}$ by $\nu^{\frac{1}{2}}$. Indeed, we can assume that $\partial A'(z) = 0$. Then γ-vicinity of z we have $\mu = O(\nu\gamma)$ and scaling we should be concerned only abut this vicinity. We select $\gamma = \nu^{-\frac{1}{2}}$.

Estimating $|\partial^2 A'|$

Recall that if A' is a minimizer, then it must satisfy (27.2.14) and then for $h^{-\frac{1}{2}} \le \beta \le h^{-1}$ due to Proposition 28.3.8(ii) $\|\Delta A'\|_{\mathscr{L}^\infty}$ does not exceed $C\kappa h^2\bigl((28.3.44)+\beta^{\frac{1}{2}} h^{-2}\bigr)$ and then $\|\partial^2 A'\|_{\mathscr{L}^\infty}$ must not exceed this expression multiplied by $C|\log h|$ plus $\|\partial A'\|_{\mathscr{L}^\infty}$ [7]:

$$\|\partial^2 A'\|_{\mathscr{L}^\infty} \le C\kappa|\log h|\bigl(\nu^{\frac{1}{2}} + (\mu+\nu h)|\log h|\bigr) \\ + C\kappa\beta h|\log h|\bigl(h^{-\frac{3}{5}}\nu^{\frac{1}{10}} + h^{-\frac{4}{7}}\nu^{\frac{1}{7}} + h^{-\frac{1}{2}}\nu^{\frac{1}{4}}|\log h|^2\bigr) + C\kappa|\log h|\beta^{\frac{1}{2}}\|\partial V\|_{\mathscr{L}^\infty} \\ + C\|\partial A'\|_{\mathscr{L}^\infty}. \tag{28.3.46}$$

Also recall that we can define $\nu := \max\bigl(\|\partial^2 A'\|_{\mathscr{L}^\infty}, 1\bigr)$; then we arrive to

Proposition 28.3.10. *Let $1 \le \beta \lesssim h^{-1}$ and* (28.3.14) *be fulfilled. Let A' be a minimizer satisfying* (28.3.15).

Then one of the following two cases holds: <u>either</u>

$$\|\partial^2 A'\|_{\mathscr{L}^\infty} \le C\mu(\kappa|\log h|^2+1) \\ + C(\kappa\beta|\log h|)^{\frac{10}{9}} h^{\frac{4}{9}} + C(\kappa\beta|\log h|)^{\frac{7}{6}} h^{\frac{1}{2}} + C(\kappa\beta|\log h|^3)^{\frac{4}{3}} h^{\frac{2}{3}} \\ + C\kappa|\log h|\omega + C\|\partial A'\|_{\mathscr{L}^\infty} \tag{28.3.47}$$

with the right-hand expressions $\ge C$ <u>or</u>

$$\|\partial^2 A'\|_{\mathscr{L}^\infty} \le C\mu(\kappa|\log h|^2+1) \\ + C\kappa\beta|\log h| h^{\frac{2}{5}} + C\kappa\beta|\log h| h^{\frac{3}{7}} + C\kappa\beta|\log h|^3 h^{\frac{1}{2}} \\ + C\kappa|\log h|\omega + C\|\partial A'\|_{\mathscr{L}^\infty} \tag{28.3.48}$$

with the right-hand expression $\le C$. Recall that ω is defined by (28.3.45).

[7] Which can be replaced by a different norm, say, $\|\partial A'\|$.

Proof. Indeed, if $\nu \ge C$ we have

$$\nu \le C\kappa\mu|\log h| + C(\kappa\beta|\log h|h^{\frac{2}{5}})^{\frac{10}{9}} + C(\kappa\beta|\log h|h^{\frac{3}{7}})^{\frac{7}{6}} + C(\kappa\beta|\log h|^3 h^{\frac{1}{2}})^{\frac{4}{3}} + C\kappa\beta^{\frac{1}{2}}\|\partial V\|_{\mathscr{L}^\infty} + C\|\partial A'\|_{\mathscr{L}^\infty},$$

which leads to (28.3.47); if $\nu \asymp 1$ we have (28.3.48). □

Remark 28.3.11. (i) Observe that the right-hand expressions of (28.3.47) and (28.3.48) are either $\lesssim 1$ or $\gtrsim 1$ simultaneously.

(ii) The second term in the right-hand expression of (28.3.47) (i.e. with the power $\frac{10}{9}$) is always greater than the third and the fourth terms unless $\kappa\beta h \ge |\log h|^{-K}$). Because of this we just take power K of $|\log h|$ in this term and skip two other terms. One can find easily that $K = 4$ is sufficient;

(iii) The second term in the right-hand expression of (28.3.47) is less than the last one as $\beta \le h^{-\frac{8}{11}}(\kappa|\log h|)^{-\frac{20}{11}}$.

(iv) Obviously, in (28.3.48) we can take $\mu = 1$; however we are missing estimate of μ in (28.3.47). For sure, we know that $\mu \le C\nu$ but we will be able to do a better work after we estimate $\|\partial A'\|^2$ in Subsubsection *28.3.5.3. Weak Magnetic Field Approach.*

28.3.4 Trace Term Asymptotics

General Microlocal Arguments

Now let us consider the trace term. We are not assuming anymore that A' is a minimizer but that it satisfies

$$\|\partial A'\|_{\mathscr{L}^\infty} \le \mu, \qquad \|\partial^2 A'\|_{\mathscr{L}^\infty} \le \nu \qquad \text{with } 1 \le \mu \le \nu \le \epsilon. \tag{28.3.49$_{1,2}$}$$

We assume that $V \in \mathscr{C}^2$ uniformly. Later we will impose on V different non-degeneracy assumptions; from now on small constant $\epsilon > 0$ in conditions (28.3.15) and (28.3.49)$_{1,2}$ depends also on the constants in the non-degeneracy assumption.

Let us introduce the scaling function

$$\ell(x) := \epsilon_0\bigl(\min_j |V - 2j\beta h| + |\partial V|^2\bigr)^{\frac{1}{2}} + \bar{\ell} \tag{28.3.50}$$

with

$$\bar{\ell} := C_0 \max\bigl(\nu\beta^{-1},\, \mu\beta^{-1},\, h^{\frac{1}{2}}\bigr). \tag{28.3.51}$$

We need the following

Proposition 28.3.12. *Let $\beta h \lesssim 1$ and $(28.3.49)_{1,2}$ be fulfilled. Consider (γ,ρ)-element with respect to (x,p_3) with $\gamma\rho\ge h$, $\gamma\le \max(\ell,\rho)$ and*

$$\rho \ge \bar{\rho} := C_0 \max\bigl(\mu\beta^{-1},\, h^{\frac{1}{2}}\bigr). \tag{28.3.52}$$

Then for

$$T_* := h\rho^{-2} \le T \le T^* := \epsilon_0 \min(1, \rho\ell^{-1}) \tag{28.3.53}$$

for (γ,ρ)-element $\{(x,\xi_3)\colon x\in B(z,\gamma), |\xi_3 - A_3(z)|\asymp \rho\}$ the following estimate

$$\begin{gathered}|F_{t\to h^{-1}\tau}\bar{\chi}_T(t)\Gamma\bigl(p_x^\alpha p_y^{\alpha'}\varphi_1(\rho^{-1}p_{3x})\varphi_2(\rho^{-1}p_{3y})\psi_1(\gamma^{-1}x)\psi_2(\gamma^{-1}y)U\bigr)|\\ \le CS(\rho,T)\gamma^3\end{gathered} \tag{28.3.54}$$

holds with

$$S(\rho,T) = \bigl(\beta h^{-1} + \rho^2 h^{-2}\bigr)\bigl(\rho^{-1} + \rho^{-3}h\nu^2\varepsilon^4 T^3\bigr), \tag{28.3.55}$$

where $\varepsilon = h\rho^{-1}$.

Observe that we redefined $\bar{\rho}$ possibly increasing it.

Proof. The proof is similar to one of Theorem 27.2.17 and is based on $h\rho^{-1}$-approximation. Note first that the propagation speed with respect to x_3 is $\asymp \rho$, the propagation speed with respect to p_3 is $O(\ell)$ and all other propagation speeds are bounded by $\bar{\rho}$. Therefore the shift with respect to x_3 is $\asymp \rho T \lesssim \ell$ as $T\le T^*$ and it is observable for $T \ge T_* = h|\log h|\rho^{-2}$ [8].

Let us apply the three-term approximation. Then since the first term does not includes any error, we can estimate it by

$$C\bigl(\beta h^{-1} + \rho^2 h^{-2}\bigr)\rho\gamma^3 h^{-1} T_* \asymp C\bigl(\beta h^{-1} + \rho^2 h^{-2}\bigr)\rho^{-1}\gamma^3,$$

[8] But in estimates we can skip the logarithmic factor using our standard scaling arguments.

which delivers the first term in $S(\rho, T)\ell^3$.

The second term is linear with respect to the perturbation $(A - A_\varepsilon)$ and asince we consider a shift by x_3 in the estimate of this term, we also can take $T = T_*$. Indeed, contributions of intervals $|t| \asymp T'$ with $T_* \le T' \le T^*$ to this term are negligible if we include a logarithmic factor in T_* [8]. Then this term does not exceed $C\bigl(\beta h^{-1} + \rho^2 h^{-2}\bigr)\rho\ell^3\nu\gamma^2 T_*^2 h^{-2}$ and it is less than the first term in $S(\rho, T)\gamma^3$.

Finally, the third term does not exceed the second term in $S(\rho, T)\gamma^3$.□

After estimate (28.3.54) has been proven we can estimate the contribution of the given element to the Tauberian error by $CS(\rho, T)\gamma^3\rho^2 h^2 T^{-2}$ [9] which is

$$C(\beta + \rho^2 h^{-1})\bigl(\rho T^{-2} + \rho^{-1}\nu^2 hT\bigr)\gamma^3. \tag{28.3.56}$$

Consider an error appearing when we replace in the Tauberian expression T by T_*. The first two terms are negligible on intervals $|t| \asymp T'$ with $T_* \le T' \le T^*$ and the third term contributes here

$$C(\beta + \rho^2 h^{-1})\rho^{-1}\nu^2 hT'\gamma^3,$$

which sums to its value for $T' = T$. Therefore this error does not exceed (28.3.56) as well.

Minimizing expression (28.3.56) by $T \le T^*$ we get

$$C(\beta + \rho^2 h^{-1})\bigl(\rho T^{*\,-2} + \rho^{-\frac{1}{3}}\nu^{\frac{4}{3}}h^{\frac{2}{3}}\bigr)\gamma^3 \asymp C(\beta + \rho^2 h^{-1})\bigl(\rho + \rho^{-1}\ell^2 + \rho^{-\frac{1}{3}}\nu^{\frac{4}{3}}h^{\frac{2}{3}}\bigr)\gamma^3, \tag{28.3.57}$$

where we do not include the last term with $T = T_*$ since then the first term would be larger than $C\beta h^{-2}\rho^3\gamma^3$, which is the trivial estimate.

Now let us sum over the partition. Observe first that

(28.3.58) The contribution of the zone $\{\rho\colon \rho \ge (\beta h)^{\frac{1}{2}}\}$ does not exceed

$$Q_0 := Ch^{-1} + Ch^{-\frac{1}{3}}\nu^{\frac{4}{3}} \tag{28.3.59}$$

since ρ here would be in the positive degree. Consider now the contribution of the zone $\{\rho\colon \rho \le (\beta h)^{\frac{1}{2}}\}$.

[9] Factors ρ^2 and $h^2 T^{-2}$ (rather than hT^{-1}) appear because we consider the trace term.

Strong Non-Degenerate Case

Here ρ is in the negative degree but we can help it under *strong non-degeneracy assumption*

$$\min_j |V-2j\beta h|+|\partial V|\ge \epsilon_0 \qquad \text{in}\quad B(0,1), \tag{28.3.60}$$

which later will be relaxed. Indeed, the relative measure of those x-balls with $\gamma=\rho^2$, where operator is non-elliptic is $\rho^2(\beta h)^{-1}$ as $\rho\ge h^{\frac{1}{3}}$. Then the total contribution of such elements does not exceed $\rho^2h^{-1}\bigl(\rho^{-1}\ell^2+\rho^{-\frac{1}{3}}\nu^{\frac{4}{3}}h^{\frac{2}{3}}\bigr)$ and the summation over ρ results in (28.3.59). Meanwhile, the total contribution of balls with $|\xi_3-A'_3|\le\bar\rho=h^{\frac{1}{3}}$ does not exceed $C\bar\rho^5h^{-3}$, which is smaller[10].

However we have another restriction, namely, $\bar\rho\ge C_0\mu\beta^{-1}$[11]. Because of this we need to increase the remainder estimate by $C\bar\rho\beta^2h^{-1}\times\bar\rho^2(\beta h)^{-1}$ i.e. by

$$Q'=\mu^3\beta^{-2}h^{-2}. \tag{28.3.61}$$

We should not be concerned about the zone $\{\rho\colon \bar\rho\ge\rho\ge(\beta h)^{\frac{1}{2}}\}$ since here we can always use $T\asymp\beta^{-1}$ and its contribution to the remainder will be the same $\mu^3\beta^{-2}h^{-2}$.

Now we need to pass from the Tauberian expression with $T=T_*$ to the magnetic Weyl expression and we need to consider only two first terms in the successive approximations. We can involve our standard methods of Section 18.9: note that $|x-y|\le c\rho T_*=C\varepsilon$ in the propagation and then we consider another unperturbed operator with $V=V(y)$ and $A'_j=A'(y)+\langle\nabla A_j(y),x-y\rangle$ frozen at point y (when we later set $x=y$). Then one can see that these terms modulo an error, not exceeding Q_0, are respectively

$$-h^{-3}\int P_{B_\varepsilon h}(V)\psi\,dx \tag{28.3.62$_1$}$$

and

$$-h^{-3}\int\bigl(P_B(V)-P_{B_\varepsilon h}(V)\bigr)\psi\,dx \tag{28.3.62$_2$}$$

---

[10] These arguments work even if $\beta\le h^{-\frac{1}{3}}$ (and therefore $(\beta h)^{\frac{1}{2}}\le h^{\frac{1}{3}}$): we just set $\gamma=h\rho^{-1}$ for $(\beta h)^{\frac{1}{2}}\le\beta\le h^{\frac{1}{3}}$.

[11] Here we can take $\mu=\|\partial A'\|_{\mathscr{L}^\infty}$ without resetting it to 1 if the former is smaller.

with $B_\varepsilon = |\nabla \times (A^0 + A'_\varepsilon)|$. Then we arrive to estimate (28.3.64) below.

Observe that non-degeneracy condition (28.3.60) was used only to estimate by $\rho^2(\beta h)^{-1}$ a relative measure of some set. However the same estimate would be achieved under slightly weaker non-degeneracy condition

$$\min_j |V-2j\beta h| + |\partial V| + |\det(\operatorname{Hess} V)| \ge \epsilon_0 \qquad \text{in}\quad B(0,1); \tag{28.3.63}$$

all arguments including transition to the magnetic Weyl expression work. Therefore under this assumption the same estimate holds and we arrive to

Proposition 28.3.13. *Let $\beta h \lesssim 1$ and conditions* $(28.3.49)_{1,2}$ *be fulfilled. Then under non-degeneracy assumptions* (28.3.60) *or* (28.3.63) *estimate*

$$|\operatorname{Tr}(H^-_{A,V}\psi) + h^{-3}\int P_{Bh}(V)\psi\,dx| \le CQ \tag{28.3.64}$$

holds with $Q=Q_0+Q'$ with Q_0 and Q' defined by (28.3.59) *and* (28.3.61).

Remark 28.3.14. We will show that for a minimizer $Q\asymp Q_0$ in both cases (and even under even weaker non-degeneracy assumption (28.3.65)).

Non-Degenerate Case

Assume now that even weaker non-degeneracy condition is fulfilled:

$$\min_j |V-2j\beta h| + |\partial V| + |\partial^2 V| \ge \epsilon_0 \qquad \text{in}\quad B(0,1). \tag{28.3.65}$$

Then the measure of the degenerate set is $\rho(\beta h)^{-\frac{1}{2}}$ but even this is sufficient to obtain the same sum from the second term. In the first term we get however extra $C\beta|\log h|$ (which is $O(h^{-1})$ provided $\beta \le (h|\log h|)^{-1}$) but we can help with this too: indeed, if we fix $\ell \ge 2\bar\ell$, then the relative measure does not exceed $\rho^2(\beta h\ell)$ and summation results in $O(h^{-1})$. We still need to consider set $\{x\colon \ell(x)\le 2\bar\ell\}$, but its contribution is obviously less than $C\beta\bar\ell|\log h|$ which in turn is $O(h^{-1}+\nu|\log h|)$ (and this is $O(h^{-1})$ for a minimizer).

However contribution of the degenerate set becomes $C\beta h^{-2}\bar\rho^3\bar\ell$ which boils down to the same expression Q'. Then we arrive to

Proposition 28.3.15. *Let $\beta h \lesssim 1$ and conditions* $(28.3.49)_{1,2}$ *be fulfilled. Then under non-degeneracy assumption* (28.3.65) *estimate* (28.3.63) *holds with $Q=Q_0+Q''$, $Q''=Q'+\nu|\log h|$ with Q_0 and Q' defined by* (28.3.59) *and* (28.3.61) *respectively.*

We leave easy details to the reader.

Degenerate Case

Let us derive a remainder estimate without any non-degeneracy assumptions. In comparison with the non-degenerate case we need to sum $\beta\rho^{-\frac{1}{3}}\nu^{\frac{4}{3}}h^{\frac{2}{3}}$ and we sum it over $\rho\ge\rho_*$, resulting in the same expression with ρ replaced by ρ_*; adding the contribution of the degenerate zone, equal to $\beta\rho_*^3$, we get $\beta\rho_*^{-\frac{1}{3}}\nu^{\frac{4}{3}}h^{\frac{2}{3}}+\beta h^{-2}\rho_*^3$, which should be minimized by $\rho_*\ge\bar\rho$, resulting in $\beta\nu^{\frac{6}{5}}h^{\frac{2}{5}}+\beta\bar\rho^3$ i.e.

$$Q'''=\beta\nu^{\frac{6}{5}}h^{\frac{2}{5}}+\beta h^{-\frac{1}{2}}+\mu^3\beta^{-2}h^{-2}+\nu|\log h|. \tag{28.3.66}$$

Thus we arrive to

Proposition 28.3.16. *Let $\beta h\lesssim 1$ and conditions* $(28.3.49)_{1,2}$ *be fulfilled. Then estimate* (28.3.63) *holds with Q replaced by $Q=Q_0+Q'''$ with Q_0 and Q''' are defined by* (28.3.59) *and* (28.3.66) *respectively.*

Remark 28.3.17. We are going to apply our results to $V=W_B^{\mathsf{TF}}+\lambda$ with chemical potential λ. We know that

(i) For $M=1$ (single nucleus case) after rescalings the non-degeneracy condition (28.3.60) is fulfilled everywhere including the *boundary zone* $\{x\colon \epsilon_0\bar r\le r(x)\le C_0\bar r\}$.

(ii) For $M\ge 2$ (multiple nuclei case) after rescalings the non-degeneracy condition (28.3.60) is fulfilled if $r(x)\le\epsilon d$ where d is the minimal distance between nuclei.

(iii) Further, for $M\ge 2$ and $B\le Z^{\frac{4}{3}}$ after rescalings the non-degeneracy condition (28.3.65) is fulfilled in the zone $\{x\colon Z^{-\frac{1}{3}}\le r(x)\le\epsilon_0\bar r\}$ where $r(x)$ is the distance to the closest nuclei and $\bar r=\min\bigl(B^{-\frac{1}{4}},\,(Z-N)_+^{-\frac{1}{3}}\bigr)$.

(iv) On the other hand, the non-degeneracy condition (28.3.63) is uncalled: while we believe that that this condition is often fulfilled while (28.3.60) fails we have no proof of this.

(v) For $M\ge 2$ in the boundary zone a more delicate scaling needs to be applied to improve remainder estimate which is possible not only because W_B^{TF} is more regular than just $\mathscr{C}^2$ but also has some special properties.

28.3.5 Endgame

Until now in this Section we assumed only that A' satisfies equation to the minimizer locally (and assumptions (28.3.14)–(28.3.15)) but now we assume that A' is a minimizer.

Upper Estimate

Let us first derive an upper estimate for E^*_κ and for this we need to pick-up some A'. First of all, we try $A'=0$ resulting in

$$\mathsf{E}^*_\kappa \le \mathcal{E}^*_0 + Ch^{-1} \le \mathcal{E}^*_\kappa + Ch^{-1} + C\kappa\beta^2$$

which is a good estimate for $\kappa\beta^2 \lesssim h^{-1}$:

$$\mathsf{E}^*_\kappa \le \mathcal{E}^*_\kappa + Ch^{-1}. \tag{28.3.67}$$

However for $\kappa\beta^2 \gtrsim h^{-1}$ we need to be more subtle. Namely, we pick up a mollified minimizer for the modified functional $\bar{\mathcal{E}}_\kappa(A')$, defined by (28.2.8). More precisely, let A' be the minimizer for $\bar{\mathcal{E}}_\kappa(A')$; then $\mathcal{E}_\kappa(A') = \mathcal{E}^*_\kappa + O(h^{-1})$.

Still it is not a good choice since our approach relies upon $\mathscr{C}^2$-smoothness but A' is only $\mathscr{C}^{\frac{3}{2}}$-smooth.

Proposition 28.3.18. *Let $\beta h \lesssim 1$ and $\kappa\beta^2 h \gtrsim 1$; let A' be a minimizer for the modified functional $\bar{\mathcal{E}}_\kappa(A')$ and let A'_ε be its ε-mollification. Then there exists $\varepsilon > 0$ such that*

$$|\partial A'_\varepsilon| \le C\mu = \kappa\beta h, \quad |\partial^2 A'_\varepsilon| \le C\nu = C\bigl(1 + (\kappa\beta)^{\frac{4}{3}} h^{\frac{2}{3}}\bigr)|\log h| \tag{28.3.68$_{1,2}$}$$

and

$$\mathcal{E}_\kappa(A'_\varepsilon) = \mathcal{E}^*_\kappa + O(h^{-1}). \tag{28.3.69}$$

Proof. From equation to A' we observe that

$$|\partial(A' - A'_\varepsilon)| \le C\kappa(\varepsilon + \beta h\varepsilon^{\frac{1}{2}}), \quad |\partial^2 A'_\varepsilon| \le C\kappa(1 + \beta h\varepsilon^{-\frac{1}{2}})|\log h| \tag{28.3.70}$$

and

$$|\mathcal{E}_\kappa(A') - \mathcal{E}_\kappa(A'_\varepsilon)| \le C(\varepsilon^2 + \beta h\varepsilon^{\frac{3}{2}})\kappa h^{-3} + C\kappa(\varepsilon + \beta h\varepsilon^{\frac{1}{2}})^2 h^{-2} \tag{28.3.71}$$

because linear with respect to $\partial(A' - A'_\varepsilon)$ terms disappear due to equation to a minimizer. Then for $\varepsilon \ge h$ the right-hand expression of (28.3.71) is $O(h^{-1} + \kappa\beta h^{-2}\varepsilon^{\frac{3}{2}})$ and we take $\varepsilon = \min\bigl(1, (\kappa\beta)^{-\frac{2}{3}} h^{\frac{2}{3}}\bigr)$ [12], resulting in $(28.3.68)_{1,2}$ and (28.3.69) since $|\partial A'| \le C\kappa\beta h$. □

Then applying Propositions 28.3.12, 28.3.15 and 28.3.16 to operator $H_{A_\varepsilon,V}$ with $A_\varepsilon = A^0 + A'_\varepsilon$ we arrive to

Proposition 28.3.19. *(i) For $\beta h \lesssim 1$ and $\kappa\beta^2 h \lesssim 1$ estimate* (28.3.67) *holds.*

(ii) For $\beta h \lesssim 1$ and $\kappa\beta^2 h \gtrsim 1$ estimate $\mathsf{E}^*_\kappa \le \mathcal{E}^*_\kappa + CQ$ holds with $Q = Q_0$ under non-degeneracy assumption (28.3.65) *and with $Q = Q_0 + Q'''$ in the general case, calculated with $\nu = \bigl(1 + (\kappa\beta)^{\frac{4}{3}} h^{\frac{2}{3}}\bigr)|\log h|$, $\bar\rho = h^{\frac{1}{2}}$, and $\bar\ell = \max(h^{\frac{1}{2}}, \beta^{-1}\nu)$.*

Indeed, for A' selected above $\mu \le \kappa\beta h$ and one can check easily that $Q' \le Q_0$. Since ν here is lesser than one derived for a minimizer of $\mathsf{E}^*_\kappa(A')$, we are happy and skip calculation of Q'''.

Lower Estimate

Estimate (28.3.63) implies that

$$\underbrace{\mathsf{Tr}(H^-_{A,V}\psi) + \kappa^{-1}h^2\|\partial A'\|^2}_{=\mathsf{E}_\kappa(A')} \ge \underbrace{-h^{-3}\int P_{Bh}(V)\psi\,dx + \kappa^{-1}h^{-2}\|\partial A'\|^2}_{=\mathcal{E}_\kappa(A')} - CQ$$

and therefore

$$\mathsf{E}^*_\kappa \ge \mathcal{E}^*_\kappa - CQ \qquad \text{with}\ \ \mathsf{E}^*_\kappa = \inf_{A'} \mathsf{E}_\kappa(A'),\quad \mathcal{E}^*_\kappa = \inf_{A'} \mathcal{E}_\kappa(A'), \tag{28.3.72}$$

where $A' = A'_\kappa$ is a minimizer of $\mathsf{E}_\kappa(A')$ and Q is defined in Propositions 28.3.12, 28.3.15 and 28.3.16 and ν is a right-hand expression of (28.3.47) or 1 whatever is larger. For a sake of simplicity we replace it by a marginally larger expression

$$\nu = (\mu + 1)(\kappa|\log h|^2 + 1) + (\kappa\beta)^{\frac{10}{9}} h^{\frac{4}{9}}|\log h|^K + \kappa\beta^{\frac{1}{2}}|\log h|; \tag{28.3.47*}$$

recall that in “old” (28.3.47) $\mu = \|\partial A'\|_{\mathcal{L}^\infty}$ or $\mu = 1$, whatever is larger, so we modified the first term here accordingly.

[12] Then $\varepsilon \gtrsim h$ due to $\kappa\beta^2 h \gtrsim 1$.

Our problem is that so far we know neither $\|\partial A'\|_{\mathcal{L}^\infty}$ nor $\|\partial A'\|$. Observe however that

$$\mathsf{E}^*_\kappa = \mathsf{E}_\kappa(A') \ge \mathsf{E}_{2\kappa}(A') + (2\kappa)^{-1}\|\partial A'\|^2 \ge \mathcal{E}^*_{2\kappa} + (2\kappa)^{-1}\|\partial A'\|^2 - CQ \\ \ge \mathcal{E}^*_\kappa(A') - C\kappa\beta^2(2\kappa)^{-1}\|\partial A'\|^2 - CQ$$

and therefore combining this with an upper estimate we arrive to estimate

$$\|\partial A'\| \le C(\kappa h^2 Q)^{\frac{1}{2}} + C\kappa\beta h, \tag{28.3.73}$$

and we have also

$$\|\partial A'\|_{\mathscr{L}^\infty} \le C\|\partial A'\|^{\frac{2}{5}} \cdot \|\partial^2 A'\|^{\frac{3}{5}}_{\mathscr{L}^\infty}. \tag{28.3.74}$$

We are going to explore what happens if

$$\nu \asymp \mu(\kappa|\log h|^2 + 1), \tag{28.3.75}$$

where the right-hand expression is the sum of all terms in (28.3.47)* containing μ.

Remark 28.3.20. (i) Observe first that remainder estimate $Q = O(\beta^2 h^{-1})$ is guaranteed and therefore $\|\partial A'\| \le C\beta h^{\frac{1}{2}}$. Then $\mu \le C\beta^{\frac{2}{5}} h^{\frac{1}{5}} \nu^{\frac{3}{5}}$ due to (28.3.74).

(ii) Further, if (28.3.75) is fulfilled, then $\mu \le \beta h^{\frac{1}{2}}|\log h|^K$ and the same estimate holds for ν and then $Q_0 \asymp h^{-1}$, $Q''' \le C\beta h^{-\frac{1}{2}}|\log h|^K$; then the rough estimate to Q is improved, and then $\mu \ll \beta h^{\frac{1}{2}}$, $\nu \ll \beta h^{\frac{1}{2}}$ and, finally, $Q \asymp h^{-1}$ under assumption (28.3.65) and $Q \asymp h^{-1} + \beta h^{-\frac{1}{2}}$ in the general case, and we also have nice estimates to μ, ν.

Therefore we can assume that (28.3.75) is not fulfilled, but then ν is defined by the remaining terms and then

$$\nu = \kappa|\log h| + \kappa \min(\beta^{\frac{3}{2}} h^{-\frac{1}{2}}, \beta^{\frac{1}{2}})|\log h| + (\kappa\beta)^{\frac{10}{9}} h^{\frac{4}{9}}|\log h|^K \tag{28.3.76}$$

(and from now we do not reset to 1 if this expression is smaller).

We *almost* proved the following estimates for Q:

(28.3.77) $Q = Q_0$ under non-degeneracy assumption (28.3.65) and $Q = Q_0 + \beta h^{-\frac{1}{2}} \asymp h^{-1} + \beta h^{-\frac{1}{2}}$ in the general case.

However we need still explore what happens if $Q \asymp \mu^3\beta^{-2}h^{-2}$. In this case $\mu \le (\mu^3\beta^{-2})^{\frac{1}{5}}\nu^{\frac{3}{5}}$ and then $\mu^{\frac{2}{5}} \le \beta^{-\frac{2}{5}}\nu^{\frac{3}{5}}$, and using (28.3.76) one can prove easily (28.3.77) unless $\beta \le h^{-\frac{1}{5}}|\log h|^K$ in which case $\nu = (\kappa|\log h| + 1)$.

Weak Magnetic Field Approach

Consider now case $\beta \lesssim h^{-\frac{1}{3}}$. Recall that then $\nu \le C\kappa|\log h|$ and $\mu \ll 1$. Then as we study propagation with respect to p_3 we do not need to correct it to p'_3 and then we do not need $\bar{\rho}$.

Then we can apply *weak magnetic field approach* (see Section 13.4). Now contribution of a partition element with $\rho \ge C_0\beta^{-1}$ does not exceed $\rho^3 h^{-1} \times \rho^{-2}$ as we use $T \le \epsilon_0 \rho$ and the total contribution of such elements does not exceed Ch^{-1}; meanwhile the total contribution of elements with $\rho = C_0\beta^{-1}$ does not exceed $C\beta^2 h^{-1} \times \beta^{-3} \le Ch^{-1}$ as we use $T = \epsilon_0\beta^{-1}$.

Main Theorem

Therefore after we plug ν into Q_0 we have proven our estimate from below and also the main theorem of this Section:

Theorem 28.3.21. *Let $\beta h \lesssim 1$ and $\kappa \le \kappa^*$. Then*

(i) Estimate

$$|\mathsf{E}^*_\kappa - \mathcal{E}^*_\kappa| \le CQ \tag{28.3.78}$$

holds where under non-degeneracy assumption (28.3.65)

$$Q := h^{-1} + \kappa^{\frac{40}{27}}\beta^{\frac{40}{27}} h^{\frac{7}{27}} |\log h|^K, \tag{28.3.79}$$

and in the general case

$$Q := h^{-1} + \beta h^{-\frac{1}{2}}. \tag{28.3.80}$$

(ii) For a minimizer the following estimate holds: $\|\partial^2 A'\|_{\mathscr{L}^\infty} \le C\nu$ with ν, defined by (28.3.76).

We leave as an easy exercise to the reader

Problem 28.3.22. (i) Starting from estimate $\|\partial^2 A'\|_{\mathscr{L}^\infty} \le C\nu$ derive from (28.3.73)–(28.3.74) estimate for $\|\partial A'\|_{\mathscr{L}^\infty}$; consider separately three cases: $1 \le \beta \le h^{-\frac{1}{3}}$, $h^{-\frac{1}{3}} \le \beta \le h^{-\frac{1}{2}}$ and $h^{-\frac{1}{2}} \le \beta \le 1$.

(ii) Prove that for $\kappa\beta^2 h \gtrsim 1$

$$\|\partial(A' - A'')\| \le C(\kappa Q h^2)^{\frac{1}{2}}, \tag{28.3.81}$$

where A' and A'' are minimizers for E_κ and $\bar{\mathcal{E}}_\kappa$ respectively; in particular, observe that $\|\partial(A' - A'')\| \ll \|\partial A'\|$ for $\kappa\beta^2 h \gg 1$;

(iii) Since (28.3.81) holds for A'' replaced by A''_ε as well and since we have estimate $\|\partial^2 A''_\varepsilon\|_{\mathscr{L}^\infty} \le C\nu$, derive from (28.3.81) estimate for $\|\partial(A' - A''_\varepsilon)\|_{\mathscr{L}^\infty}$ and then the same estimate for $\|\partial A'\|_{\mathscr{L}^\infty}$.

Remark 28.3.23. In the following observations we use simpler but less sharp upper estimates to critical β:

(i) Under non-degeneracy assumption (28.3.65) we conclude that $Q \le Ch^{-1}$ and $\nu \le C\beta^{\frac{1}{2}}|\log h|$ for $\beta \le h^{-\frac{2}{3}}$ and therefore $\mu \le 1$ for $\beta \le h^{-\frac{2}{3}}|\log h|^{-K}$.

(ii) In the general case we see that $Q \le Ch^{-1} + C\beta h^{-\frac{1}{2}}$ and $\nu \le C\beta^{\frac{1}{2}}|\log h|$ for $\beta \le h^{-\frac{2}{3}}$ and therefore $\mu \le 1$ fors $\beta \le h^{-\frac{3}{5}}|\log h|^{-K}$; we used here estimate $\mu \le C(\kappa h^2 Q)^{\frac{1}{5}}\nu^{\frac{3}{5}}$.

28.3.6 N-Term Asymptotics

Introduction

In the application to the ground state energy one needs to consider also N-term asymptotics and D-term estimates. Let us start from the former: we consider N-term

$$\int e(x,x,0)\psi(x)\,dx. \tag{28.3.82}$$

Again we consider this asymptotics in the more broad content of assumptions $V \in \mathscr{C}^2$ and $(28.3.49)_{1,2}$ and we will follow arguments employed for a trace term using the same notations. Then the Tauberian error does not exceed $CS(\rho, T)\gamma^3 hT^{-1}$[13], which is

$$C(\beta + \rho^2 h^{-1})h^{-1}\bigl(\rho^{-1}T^{-1} + \rho^{-3}\nu^2 hT^{-2}\bigr)\gamma^3. \tag{28.3.56$'$}$$

[13] With $S(\rho, T)$ defined by (28.3.28).

Minimizing by $T \le T^*$ we get

$$C(\beta+\rho^2 h^{-1})h^{-1}\bigl(\rho^{-1}+\rho^{-2}\ell+\rho^{-\frac{5}{3}}\nu^{\frac{2}{3}}h^{\frac{1}{3}}\bigr)\gamma^3. \tag{28.3.57$'$}$$

Then summation over zone $\{\rho\colon \rho^2\ge \beta h\}$ results in

$$R_0 = C(h^{-2}+h^{-\frac{5}{3}}\nu^{\frac{2}{3}}) \tag{28.3.59$'$}$$

and we need to consider only contributions of elements belonging to the zone $\{\rho\colon \rho^2\le \beta h\}$

$$\beta h^{-1}\bigl(\rho^{-1}+\rho^{-2}\ell+\rho^{-\frac{5}{3}}\nu^{\frac{2}{3}}h^{\frac{1}{3}}\bigr)\gamma^3. \tag{28.3.83}$$

Strong Non-Degenerate Case

Under non-degeneracy conditions (28.3.60) or (28.3.63) expression (28.3.83) should be multiplied by $\rho^2(\beta h)^{-1}\gamma^{-3}$ and after summation by ρ we get an extra term $Ch^{-2}|\log h|$.

However we can get rid of the logarithmic factor by the standard trick: in one direction time could be improved to $\rho^{1-\delta}\ell^\delta$. We leave easy details to the reader.

Further, adding $R' = C\beta h^{-2}\bar\rho\times\bar\rho^2(\beta h)^{-1}$ with $\bar\rho = C_0\max(\mu\beta^{-1},\ h^{\frac{1}{2}})$ [11)] i.e.

$$R' = \mu^3\beta^{-3}h^{-3}, \tag{28.3.61$'$}$$

which is a contribution of the zone $\{\rho\colon \rho\le\bar\rho\}$, we arrive to

Proposition 28.3.24. *Let $\beta h\lesssim 1$ and conditions* (28.3.49)$_{1,2}$ *be fulfilled. Then under non-degeneracy assumption* (28.3.60) *or* (28.3.63) *estimate*

$$|\int \bigl(\operatorname{tr} e(x,x,0) - h^{-3}\int P'_{Bh}(V)\bigr)\psi(x)\,dx| \le CR \tag{28.3.84}$$

holds with $R=R_0+R'$, R_0, R' defined by (28.3.59)$'$ *and* (28.3.61)$'$.

Remark 28.3.25. The above estimate is sufficiently good since the weak magnetic field approach brings remainder estimate $C\mu h^{-2}$ even without any non-degeneracy assumption. We leave easy details to the reader.

Non-Degenerate Case

Under non-degeneracy assumption (28.3.65) we need to apply more subtle arguments than before. Consider first subelements[14)] with $\rho\ge \ell$; for them we need to multiply expression (28.3.83) by $\rho\gamma^{-3}$ and sum by $\rho\ge\rho_*$, resulting in $C\beta h^{-1}|\log h| + C\beta h^{-\frac{2}{3}}\nu^{\frac{2}{3}}\rho_*^{-\frac{2}{3}}$.

On the other hand, for subelements with $\rho\le \ell$ we need to multiply (28.3.83) by $\rho^2(\beta h)^{-1}\gamma^{-3}$ and sum by $\rho_*\le\rho\le \ell$ and then by $\ell\ge \rho_*$, resulting in the same expression albeit with a factor $|\log h|^2$ instead of $|\log h|$. Here we get also $Ch^{-2}|\log h|$ term but we deal with it exactly as in the previous Subsubsection *28.3.6.2 Strong Non-Degenerate Case.*

We need also to add contributions of subelements with $\rho_*\le \rho\le \ell\le \bar{\ell}$ and with $\rho\le\rho_*$. For the former subelements we need to consider only term $\beta h^{-1}\rho^{-2}\bar{\ell}\gamma^3$ in (28.3.83) and only if $\bar{\ell}=\nu\beta^{-1}$, resulting in $\beta h^{-1}\rho_*^{-1}\bar{\ell}\gamma^3$ and contribution of the latter subelements we estimate by $\beta h^{-2}\rho_*^2$. So we get

$$C\beta\bigl(h^{-1}|\log h| + h^{-1}\rho_*^{-1}\bar{\ell} + h^{-\frac{2}{3}}\nu^{\frac{2}{3}}\rho_*^{-\frac{2}{3}} + h^{-2}\rho_*^2\bigr),\tag{28.3.85}$$

which should be minimized by $\rho_*\ge\bar{\rho}$, resulting in

$$C\beta\bigl(h^{-1}|\log h|^2 + h^{-\frac{4}{3}}\bar{\ell}^{\frac{2}{3}} + h^{-1}\nu^{\frac{1}{2}} + h^{-2}\bar{\rho}^2\bigr).$$

Then plugging $\bar{\rho}$ and $\bar{\ell}=\nu\beta^{-1}$ we arrive to

$$R'' = C\beta\bigl(h^{-1}|\log h|^2 + h^{-\frac{4}{3}}\nu^{\frac{2}{3}}\beta^{-\frac{2}{3}} + h^{-1}\nu^{\frac{1}{2}}\bigr) + C\mu^2\beta^{-1}h^{-2}\tag{28.3.86}$$

thus proving Proposition 28.3.26(i) below.

Degenerate cCase

In the general case we arrive to (28.3.85) albeit with factor ρ_*^{-1}

$$C\beta\bigl(h^{-1}\rho_*^{-1} + h^{-1}\rho_*^{-2}\bar{\ell} + h^{-\frac{2}{3}}\nu^{\frac{2}{3}}\rho_*^{-\frac{5}{3}} + h^{-2}\rho_*\bigr),\tag{28.3.87}$$

which should be minimized by $\rho_*\ge\bar{\rho}$, resulting in

$$C\beta\bigl(h^{-\frac{3}{2}} + h^{-\frac{5}{3}}\bar{\ell}^{\frac{1}{3}} + h^{-\frac{4}{3}}\nu^{\frac{1}{4}} + h^{-2}\bar{\rho}\bigr).$$

[14)] We call them "subelements" but they live in the phase spaces in contrast to elements which live in the coordinate spaces.

Then plugging $\bar\rho$ and $\bar\ell$ we arrive to

$$R''' = C\beta\bigl(h^{-\frac{3}{2}} + h^{-\frac{5}{3}}\nu^{\frac{1}{3}}\beta^{-\frac{1}{3}} + h^{-\frac{4}{3}}\nu^{\frac{1}{4}}\bigr) + C\mu h^{-2} \tag{28.3.88}$$

thus proving Proposition 28.3.26(ii):

Proposition 28.3.26. *Let $\beta h \lesssim 1$ and conditions* (28.3.49)$_{1,2}$ *be fulfilled. Then*

(i) Under non-degeneracy assumption (28.3.65) *estimate* (28.3.63) *holds with $R = R_0 + R''$, R_0, R'' defined by* (28.3.59)$'$ *and* (28.3.86).

(ii) In the general case estimate (28.3.63) *holds with $R = R_0 + R'''$, R_0, R''' defined by* (28.3.59)$'$ *and* (28.3.88).

28.3.7 D-Term Estimate

Consider now D-term

$$\mathsf{D}\bigl([e(x,x,0) - h^{-3}P'_{Bh}(V)]\psi,\ [e(x,x,0) - h^{-3}P'_{Bh}(V)]\psi\bigr) \tag{28.3.89}$$

with $\psi \in \mathscr{C}_0^\infty((B(0,1))$.

Proposition 28.3.27. *Let $\beta h \lesssim 1$ and A' satisfy* (28.3.49)$_{1,2}$. *Then under non-degeneracy assumption* (28.3.60) D*-term* (28.3.89) *does not exceed CR^2 with $R = R_0 + R'$, R_0 and R' defined by* (28.3.59)$'$ *and* (28.3.61)$'$.

Proof. *Step 1.* Let us apply Fefferman-de Llave decomposition (16.4.1); then we need to consider pairs of elements $B(\bar x, r)$ and $B(\bar y, r)$ such that $3r \le |\bar x - \bar y| \le 4r$. If $r \ge \bar\rho$, then on each of these elements we should consider (γ, ρ) subelements (we call them "subelements" but they live in the phase spaces in contrast to the elements which live in the coordinate spaces). Then we have three parameters, namely (r, ρ_x, ρ_y).

Observe that for each $\bar y$ the number of matching x-elements is $\asymp 1$ and that the summation with respect to $\rho_x \ge \rho^* = (\beta h)^{\frac{1}{2}}$ results in $R_0 r^2$ multiplied by a contribution of (γ, ρ_y)-subelement; after summation by r and then by these (γ, ρ_y)-subelements we get CR_0R. Similarly we are dealing with $\rho_y \ge \rho^*$.

Therefore we need to consider only the case when both ρ_x and ρ_y do not exceed ρ^*. If $r \ge c\rho^*$, then "the relative measure trick" allows us to add factors $\rho_x^2(\beta h)^{-1}$ and $\rho_y^2(\beta h)^{-1}$ even if $\rho_x^2 \ge r$ or $\rho_y^2 \ge r$ and then the total contribution of such subelements also does not exceed CR^2.

Step 2. Consider next $h \le r \le \rho^{*}$ [15] and we should look only at $\rho_x \le \rho^*$, $\rho_y \le \rho^*$. Further, if $\rho_x^2 \ge \epsilon r$ or $\rho_y^2 \ge \epsilon r$ we can always inject factor $c\rho_x^2 r^{-1}$ or $c\rho_y^2 r^{-1}$ ending up again with CR^2.

On the other hand, if both $\rho_x^2 \le \epsilon r$ and $\rho_y^2 \le \epsilon r$ but $r \ge c\bar{\rho}$ we can apply the same "relative measure trick" but comparing the measure of ρ_x^2- or ρ_y^2-elements with violated ellipticity assumption to the total measure of $B(z,r)$; then we can inject factors $(\rho_x^2/r)^\theta$ and $(\rho_y^2/r)^\theta$ with arbitrary $0 \le \theta \le 1$ and we select any $\theta : \frac{5}{6} < \theta < 1$ to have positive powers of ρ_x and ρ_y and power of r (counting r^{-1}) greater than -3. We end up again with CR^2.

Observe that these arguments cover also cases $\rho_x \le \bar{\rho}$ or $\rho_y \le \bar{\rho}$.

Step 3. To estimate the contribution of zone $\{(x,y)\colon r \le h\}$ we just estimate $|e(x,x,\tau)| \le Ch^{-3}$. □

For $M \ge 2$ we will need to estimate D-term under non-degeneracy assumptions (28.3.63), or (28.3.65), or without any non-degeneracy assumption.

Proposition 28.3.28. *Let $\beta h \lesssim 1$ and A' satisfy* (28.3.49)$_{1,2}$. *Then* D*-term* (28.3.89) *does not exceed CR^2 where*

(i) Under non-degeneracy assumption (28.3.63) $R = R_0 + R'$, R_0 *and* R' *defined by* (28.3.59)$'$ *and* (28.3.61)$'$.

(ii) Under non-degeneracy assumption (28.3.65) $R = R_0 + R''$, R_0 *and* R'' *defined by* (28.3.59)$'$ *and* (28.3.86).

(iii) In the general case $R = R_0 + R'''$, R_0 *and* R''' *defined by* (28.3.59)$'$ *and* (28.3.88).

Proof. Let us use ideas used in the proofs of Proposition 28.3.26, 28.3.24 and 28.3.26. Let us apply Fefferman-de Llave decomposition (16.4.1); then we need to consider pairs of elements $B(\bar{x},r)$ and $B(\bar{y},r)$ with $3r \le |\bar{x}-\bar{y}| \le 4r$. If $r \ge \bar{\rho}$ on each of these elements we should consider (γ,ρ) subelements[14]. Then again we have three parameters, namely (r,ρ_x,ρ_y). On the other hand, there is a scaling function $\ell(x)$ and covering of $B(0,1)$ by ℓ-elements.

[15] Observe that we do not need to keep $t \ge \bar{\rho}$ but we need to keep $\rho r \ge h$.

Part 1. Consider case of $\ell_x\lesssim r$ (and therefore $\ell_y\lesssim r$). Then we must assume that $\rho_x\ell_x\gtrsim h$, $\rho_y\ell_y\gtrsim h$. Observe as in *Step 1* of the previous proof that if $\rho_x\gtrsim \rho^*=(\beta h)^{\frac{1}{2}}$, then the relative density of such subelements is $\rho_x^2/(\beta h)$ and therefore the summation over such subelements of the given x-element results in $CR_0\ell_x^3$. Therefore the double summation over corresponding subelements of x- and y-elements results in $CR_0^2\ell_x^3\ell_y^3 r^{-1}$. Finally, after the double summation over x- and y-elements we get $CR_0^2\int |x-y|^{-1}\,dxdy$, which does not exceed CR_0^2.

Therefore in what follows we need to consider only subelements with $\rho_x\lesssim\rho^*$, $\rho_y\lesssim\rho^*$ [16]. Further, observe that the same arguments are applicable if $\ell_x\gtrsim\rho^*$, $\ell_y\gtrsim\rho^*$ and we are left with the pairs of elements with $\ell_x\lesssim\rho^*$, $\ell_y\lesssim\rho^*$ and their subelements with $\rho_x\lesssim\rho^*$, $\rho_y\lesssim\rho^*$ since we will always keep $\ell_x\ge\bar\rho$, $\ell_y\ge\bar\rho$.

Observe that the summation of (28.3.83) over subelements with $\rho\ge\ell$ of the given element results in

$$C\beta h^{-1}\bigl(\ell^{-1}+\ell^{-\frac{5}{3}}\nu^{\frac{2}{3}}h^{\frac{1}{3}}\bigr)\ell^3. \tag{28.3.90}$$

On the other hand, for $\rho\le\ell$ the relative density of ρ-subelements of the given ℓ-element does not exceed $C\rho^2\ell^{-2}$ and therefore summation over such subelements results in (28.3.90) again.

However in (28.3.83) if $\ell\le\bar\ell$ we need to take in the middle term $\ell=\bar\ell$ and here we can ignore other options but $\bar\ell=\nu\beta^{-1}$.

Then the summation of this term over subelements with $\rho\ge\max(\ell,\rho_*)$ results in $C\beta h^{-1}\min(\rho_*^{-2},\ell^{-2})\bar\ell\ell^3$ and the summation over subelements with $\rho_*\le\rho\le\ell$ results in $C\beta h^{-1}\rho_*^{-2}\bar\ell(1+|\log\rho_*\ell^{-1}|)\ell^3$ (and should be counted as $\ell\ge\rho_*$ only.

Finally, the contribution of subelements with $\rho\le\rho_*$ does not exceed $C\beta h^{-2}\rho_*^3\ell$ and $C\beta h^{-2}\rho_*\ell^3$ if $\rho_*\le\ell$ and $\rho_*\ge\ell$ respectively. So, in the former case the total contribution of all subelements does not exceed

$$C\beta h^{-1}\Bigl[\ell^{-1}+\ell^{-\frac{5}{3}}\nu^{\frac{2}{3}}h^{\frac{1}{3}}+\rho_*^{-2}\bar\ell(1+|\log\rho_*\ell^{-1}|)+h^{-1}\rho_*^3\ell^{-2}\Bigr]\ell^3. \tag{28.3.91}$$

[16] Due to positivity quadratic form $\mathsf{D}(.,.)$ we need to consider only “pure” pairs. We will use this observation many times.

Minimizing this expression by ρ_* we get

(28.3.92)
$$C\beta h^{-1}\Bigl[\ell^{-1}+\nu^{\frac{2}{3}}h^{\frac{1}{3}}\ell^{-\frac{5}{3}}+\bar{\ell}^{\frac{3}{5}}h^{-\frac{2}{5}}(1+|\log \ell_*\ell^{-1}|)^{\frac{3}{5}}\ell^{-\frac{4}{5}}+h^{-1}\bar{\rho}^3\ell^{-2}\Bigr]\ell^3,$$

achieved for

(28.3.93)
$$\rho_*=\rho_*(\ell)\asymp \max((\bar{\ell}h\ell^2|\log h|)^{\frac{1}{5}},\bar{\rho})\qquad \text{if}\quad \ell\ge \ell_*=\max((\bar{\ell}h|\log h|)^{\frac{1}{3}},\ \bar{\rho}).$$

Then N-term does not exceed

(28.3.94)
$$C\beta h^{-1}\int_{\ell_x\ge\ell_*}\Bigl[\ell_x^{-1}+\nu^{\frac{2}{3}}h^{\frac{1}{3}}\ell_x^{-\frac{5}{3}}+\bar{\ell}^{\frac{3}{5}}h^{-\frac{2}{5}}(1+|\log \ell_*\ell_x^{-1}|)^{\frac{3}{5}}\ell_x^{-\frac{4}{5}}+h^{-1}\bar{\rho}^3\ell_x^{-2}\Bigr]\,dx+\\ C\beta h^{-1}\Bigl[\ell_*^{-1}+\nu^{\frac{2}{3}}h^{\frac{1}{3}}\ell_*^{-\frac{5}{3}}+\bar{\ell}^{\frac{3}{5}}h^{-\frac{2}{5}}\ell_*^{-\frac{4}{5}}+h^{-1}\bar{\rho}^3\ell_*^{-2}\Bigr]\,\mathsf{mes}(\{\ell_x\le\ell_*\})$$

where the first and second terms estimate contributions of elements with $\ell_x\ge\ell_*$ and $\ell_x\le\ell_*$ respectively.

Remark 28.3.29. Observe that

(i) Under non-degeneracy assumption (28.3.60) we get $C(R_0+R')$ as expected and under non-degeneracy assumption (28.3.63) we get $C(R_0+R'|\log h|)$ but this is only because we counted here the contribution of subelements with $\{x\colon \rho_x\le\ell_x\}$ in the less efficient way.

(ii) Under non-degeneracy assumption (28.3.65) we get $C(R_0+R'')$ and and in the general case we get $C(R_0+R''')$ where R_0,R',R'',R''' are defined in Propositions 28.3.24 and 28.3.26.

Similarly, the total contribution of the zone considered here (in *Part I*) to D-term does not exceed

(28.3.95)
$$C\beta^2h^{-2}\iint_{\ell_x\ge\ell_*,\ell_y\ge\ell*,|x-y|\ge\max(\ell_x,\ell_y)}$$

$$\times \Bigl[\ell_x^{-1}+\nu^{\frac{2}{3}}h^{\frac{1}{3}}\ell_x^{-\frac{5}{3}}+\bar{\ell}^{\frac{3}{5}}h^{-\frac{2}{5}}(1+|\log \ell_*\ell_x^{-1}|)^{\frac{3}{5}}\ell_x^{-\frac{4}{5}}+h^{-1}\bar{\rho}^3\ell_x^{-2}\Bigr]$$
$$\times \Bigl[\ell_y^{-1}+\nu^{\frac{2}{3}}h^{\frac{1}{3}}\ell_y^{-\frac{5}{3}}+\bar{\ell}^{\frac{3}{5}}h^{-\frac{2}{5}}(1+|\log \ell_*\ell_y^{-1}|)^{\frac{3}{5}}\ell_y^{-\frac{4}{5}}+h^{-1}\bar{\rho}^3\ell_y^{-2}\Bigr]$$
$$\times\ |x-y|^{-1}\,dxdy$$
$$+C\beta^2h^{-2}\Bigl[\ell_*^{-1}+\nu^{\frac{2}{3}}h^{\frac{1}{3}}\ell_*^{-\frac{5}{3}}+\bar{\ell}^{\frac{3}{5}}h^{-\frac{2}{5}}\ell_*^{-\frac{4}{5}}+h^{-1}\bar{\rho}^3\ell_*^{-2}\Bigr]^2\iint_{\ell_x\le\ell_*,\ell_y\le\ell*}|x-y|^{-1}\,dxdy.$$

Then under non-degeneracy assumption (28.3.60) we get $C(R_0+R')^2$ as expected while under weaker non-degeneracy assumption (28.3.63) we get $C(R_0+R'|\log h|)^2$ but this is only because we counted here contribution of subelements with $\{x\colon \rho_x\le\ell_x\}$ in the less efficient way. Using the method employed in the proof of Proposition 28.3.24 we can recover estimate $C(R_0+R')^2$ as well.

Further, under non-degeneracy assumption (28.3.63) we get $C(R_0+R'')^2$ and under non-degeneracy assumption (28.3.65) we get $C(R_0+R''')^2$.

Part 2. Consider the case of $\ell_x\ge Cr$ (and therefore $\ell_y\asymp\ell_x$). Then we apply the same arguments as before albeit with ℓ^2 replaced by ℓr. First, consider the pair of subelements with $\rho_x\ge\rho^*$, $\rho_y\ge\rho^*$. Their contribution to D-term does not exceed the product of expressions (28.3.83) with $\rho=\rho_x$, $\gamma=\gamma_x$ multiplied by $\rho_x^2(\beta h)^{-1}$ and (28.3.83) with $\rho=\rho_y$, $\gamma=\gamma_y$ multiplied by $\rho_x^2(\beta h)^{-1}$, and multiplied by $|x-y|^{-1}$. Then the double summation by ρ_x, ρ_y results in $Ch^{-4}(1+\nu^{\frac{4}{3}}h^{\frac{2}{3}})\gamma_x^3\gamma_y^3|x-y|^{-1}$; and, finally, the double summation over x, y returns $Ch^{-4}(1+\nu^{\frac{4}{3}}h^{\frac{2}{3}})\iint|x-y|^{-1}\,dxdy\lesssim CR^2$.

Then we need to consider pairs with $\rho_x\le\rho^*$, $\rho_y\le\rho^*$ and also pairs with $|x-y|\le h\max(\rho_x^{-1},\rho_y^{-1})$.

Next consider pairs of subelements with $\rho^*\ge\rho_x\ge(\ell r)^{\frac{1}{2}}$, $\rho^*\ge\rho_y\ge(\ell r)^{\frac{1}{2}}$. Their contributions to D-term does not exceed expression

$$C\beta^2h^{-2}\bigl(\rho_x^{-1}\rho_y^{-1}+\bar{\ell}^2\rho_x^{-2}\rho_y^{-2}+\rho_x^{-\frac{5}{3}}\rho_y^{-\frac{5}{3}}\nu^{\frac{4}{3}}h^{\frac{2}{3}}\bigr)\,\underbrace{\gamma_x^3\gamma_y^3|x-y|^{-1}}$$

and the double summation over x,y in $B(z,\ell)$ with $\ell_z=\ell$ results in the same expression with the selected factor replaced by ℓ^5 and then the double summation over ρ_x, ρ_y results in

$$C\beta^2h^{-2}\Bigl[\ell^{-2}+\bar{\ell}^2\ell^{-4}+\ell^{-\frac{10}{3}}\nu^{\frac{4}{3}}h^{\frac{2}{3}}\Bigr]\ell^5.\tag{28.3.96}$$

Meanwhile, considering pairs of subelements with $(\ell r)^{\frac{1}{2}} \ge \rho_x \ge \rho_*$ and $(\ell r)^{\frac{1}{2}} \ge \rho_y \ge \rho_*$ (we use $\rho_* = \rho_*(\ell)$ and ℓ_* introduced in (28.3.93)) we gain factor $\rho_x^2\rho_y^2/(\rho\ell)$ in the summation by subelements and we arrive to the same expression (28.3.96) but with a logarithmic factor at $\bar{\ell}^2$:

$$C\beta^2 h^{-2}\Bigl[\ell^{-2} + \bar{\ell}^2\ell^{-4}(1+|\log \rho_*\ell^{-1}|)^3 + \ell^{-\frac{10}{3}}\nu^{\frac{4}{3}}h^{\frac{2}{3}}\Bigr]\ell^5.$$

However we can get rid of logarithmic factors exactly as in the proof of Proposition 28.3.26 thus getting (28.3.96). Then we need to sum by balls $B(z,\ell_z)$ resulting in the same expression multiplied by ℓ^{-3} and integrated:

$$C\beta^2 h^{-2}\int_{\{\ell_x\ge \ell_*\}} \Bigl[\ell_x^{-2} + \bar{\ell}^2\ell_x^{-4} + \ell_x^{-\frac{10}{3}}\nu^{\frac{4}{3}}h^{\frac{2}{3}}\Bigr]\ell_x^2\, dx,$$

which we estimate by

$$C\beta^2 h^{-2}\int_{\ell\ge \ell_*} \Bigl[\ell^{-2} + \bar{\ell}^2\ell^{-4} + \ell^{-\frac{10}{3}}\nu^{\frac{4}{3}}h^{\frac{2}{3}}\Bigr]\ell^{2+m}\, d\ell \tag{28.3.97}$$

with $m=2,1,0$ under non-degeneracy assumptions (28.3.63), (28.3.65) and in the general case respectively. Then we arrive to the terms of integrand multiplied by ℓ and calculated either for $\ell=1$ or $\ell=\ell_*$. One can see easily that this does not exceed CR^2 with R defined in the corresponding statement of Proposition 28.3.24.

One also can derive easily the same estimate for contributions of the pairs of subelements with $\rho_x\le \rho_*(\ell)$, $\rho_y \le \rho_*(\ell)$, $\ell\ge \ell_*$, and for contributions of the pairs of subelements with $\rho_x\le \ell_*$, $\rho_y\le \ell_*$, $\ell \le \ell_*$, assuming in both cases that $\rho_x r\ge h$, $\rho_y r \ge h$.

Finally, like in the proof of Proposition 28.3.26 we estimate the contribution of zone $\{x,y\colon \rho_x r\le h,\ \rho_y r\le h\}$. We leave easy details to the reader.
□

Remark 28.3.30. These arguments also work to estimate

$$\mathsf{D}\bigl(\Gamma_x(hD-A)_x\cdot \boldsymbol{\sigma} e(.,.,0),\, \Gamma_x\bigl(hD-A)_x\cdot \boldsymbol{\sigma} e(.,.,0)\bigr). \tag{28.3.98}$$

Indeed, Weyl expression for $\Gamma_x(hD-A)_x\cdot\boldsymbol{\sigma} e(.,.,0)$ is just 0. Therefore we arrive under either of non-degeneracy assumptions (28.3.60), (28.3.63), (28.3.65) and in the general case to estimate

$$\|\nabla A'\| \le C\kappa h^2 R, \tag{28.3.99}$$

which could be better or worse than estimate $\|\nabla A'\| \le C\kappa^{\frac{1}{2}}$ which we have already. It is not clear if estimate $\|\nabla A'\| \le C\kappa$ holds.

28.4 Microlocal Analysis: $\beta h \gtrsim 1$

Now let us investigate the case of $\beta h \gtrsim 1$. In this case we assume not only that $\kappa \lesssim 1$ but also (28.2.27)*: $\kappa\beta h^2|\log h|^K \le 1$. We can apply the same arguments as before and in the end of the day we will get the series of the statements; we leave most of the easy details to the reader.

28.4.1 Estimate to a Minimizer

Observe first that

$$\|\partial A'\|^2 \le C\beta h^{-2} \times \kappa h^2 = C\kappa\beta \le Ch^{-2}|\log h|^{-K} \tag{28.4.1}$$

and

$$|\Delta A'| \le C\beta h^{-2} \times \kappa h^2 = C\kappa\beta \le Ch^{-2}|\log h|^{-K},$$

and therefore

$$|\partial^2 A'| \le C\kappa\beta \le Ch^{-2}|\log h|^{-K}. \tag{28.4.2}$$

First of all, repeating arguments leading to Proposition 28.4.8, we arrive to estimate (28.3.46) modified

$$\begin{aligned}\|\partial^2 A'\|_{\mathscr{L}^\infty} \le C\kappa \underbrace{\beta h}\nu^{\frac{1}{2}}|\log h|^2 \\ + C\kappa\beta h|\log h|\bigl(\underbrace{h^{-\frac{3}{5}}\nu^{\frac{1}{10}}} + \underbrace{h^{-\frac{4}{7}}\nu^{\frac{1}{7}}} + h^{-\frac{1}{2}}\nu^{\frac{1}{4}}|\log h|^2\bigr) + C\kappa|\log h|\beta^{\frac{1}{2}}\|\partial V\|_{\mathscr{L}^\infty} \\ + C\|\partial A'\|_{\mathscr{L}^\infty}.\end{aligned} \tag{28.4.3}$$

Note a new factor βh in the first line, which first becomes

$$C\kappa\beta h|\log h|\bigl(\nu^{\frac{1}{2}} + (\mu + \nu h)|\log h|\bigr). \tag{28.4.4}$$

We prove it first for $\mu = 1$ and then rescale and in virtue of Remark 28.3.9(ii) we can always replace μ by $\nu^{\frac{1}{2}} \ll h^{-1}$; then, using $\nu := \max\bigl(\|\partial^2 A'\|_{\mathscr{L}^\infty}, 1\bigr)$ and assumption (28.2.27)*, we reduce (28.4.4) to its final form in (28.4.3).

Further, under additional super-strong non-degeneracy assumption

$$\min_{x,j\ge 0} |V - 2j\beta h| \asymp 1 \tag{28.4.5}$$

we can skip two selected terms in the second line of (28.4.3), arriving to

$$\|\partial^2 A'\|_{\mathscr{L}^\infty} \le C\kappa\beta h\nu^{\frac{1}{2}}|\log h|^2 + C\kappa\beta h^{-\frac{1}{2}}\nu^{\frac{1}{4}}|\log h|^3 + C\kappa|\log h|\beta^{\frac{1}{2}}\|\partial V\|_{\mathscr{L}^\infty} + C\|\partial A'\|_{\mathscr{L}^\infty}. \tag{28.4.6}$$

Then we arrive to the following assertion:

Proposition 28.4.1 [17]**.** *Let* $\beta h \gtrsim 1$, $\kappa \le \kappa^*$ *and* (28.2.27)* *be fulfilled; let* $V \in \mathscr{C}^2$*; then*

(i) The following estimates hold:

$$\|\partial^2 A'\|_{\mathscr{L}^\infty} \le \nu \tag{28.4.7}$$

with

$$\nu := C\kappa\beta^{\frac{1}{2}}|\log h| + C(\kappa\beta)^{\frac{10}{9}}h^{\frac{4}{9}}|\log h|^K \qquad \textit{for } \kappa\beta h \le 1 \tag{28.4.8}$$

and

$$\nu := C\kappa\beta^{\frac{1}{2}}|\log h| + C(\kappa\beta)^{\frac{4}{3}}h^{\frac{2}{3}}|\log h|^K \qquad \textit{for } \kappa\beta h \ge 1. \tag{28.4.9}$$

(ii) Moreover, under assumption (28.4.5) *estimate* ν *is given by* (28.4.9) *even for* $\kappa\beta h \lesssim 1$.

Remark 28.4.2. (i) While case $\beta h \asymp 1$ has been already explored, we missed an important case when non-degeneracy assumption (28.4.5) is fulfilled; so we reexamine this case.

(ii) While technically (28.4.3) and (28.4.6) hold even if assumption (28.2.27)* fails provided $\nu \le \epsilon\beta$, we cannot guarantee in this case that this inequality holds.

28.4.2 Trace Term Asymptotics

Further, continuing our analysis we arrive to the following assertion

Proposition 28.4.3 [18]**.** *Let* $\beta h \gtrsim 1$, $\kappa \le \kappa^*$ *and* $\nu h^2 \le 1$ [19]*. Then*

[17] Cf. Proposition 28.3.10.

[18] Cf. Propositions 28.3.13, 28.3.15 and 28.3.16; only factor βh appears in the definition of Q_0.

[19] In the framework of Proposition 28.4.1 for a minimizer this assumption is due to (28.2.27)*.

(i) Under non-degeneracy assumption (28.3.60)*, or* (28.3.63) *remainder estimate*

$$|\operatorname{Tr}(H^-_{A,V}\psi) + h^{-3}\int P_{Bh}(V)\psi\,dx| \le Q \tag{28.4.10}$$

holds with $Q = Q_0 + Q'$,

$$Q_0 := C\beta + C\beta\nu^{\frac{4}{3}}h^{\frac{2}{3}}, \tag{28.4.11}$$

and Q' *defined by* (28.3.61)*.*

(ii) Under non-degeneracy assumption (28.3.65) *remainder estimate* (28.4.10) *holds with* $Q = Q_0 + Q''$ *with* $Q'' = Q' + \nu|\log h$ *and* Q_0 *and* Q' *defined by* (28.4.10) *and* (28.3.61) *respectively.*

(iii) In the general case remainder estimate (28.4.10) *holds with* $Q = Q_0 + Q'''$ *with* Q_0 *and* Q''' *defined by* (28.4.10) *and* (28.3.66) *respectively.*

Applying Proposition 28.4.1 we arrive to

Corollary 28.4.4. *In the framework of Proposition 28.4.3 let* A' *be a minimizer. Then*

(i) Under non-degeneracy assumption (28.3.60)*, or* (28.3.63)*, or even* (28.3.65) *estimate* (28.4.10) *holds with*

$$Q = Q_0 = C\beta + C\kappa^{\frac{40}{27}}\beta^{\frac{67}{27}}h^{\frac{34}{27}}|\log h|^K \qquad \text{for}\ \ \kappa\beta h \le 1 \tag{28.4.12}$$

and

$$Q = Q_0 = C\beta + C\kappa^{\frac{16}{9}}\beta^{\frac{25}{9}}h^{\frac{14}{9}}|\log h|^K \qquad \text{for}\ \ \kappa\beta h \ge 1. \tag{28.4.13}$$

(ii) Furthermore, under assumption (28.4.5) Q_0 *is defined by* (28.4.13) *even for* $\kappa\beta h \le 1$*.*

(iii) In the general case estimate (28.4.10) *holds with*

$$Q = Q_0 + \beta h^{-\frac{1}{2}} + \kappa^{\frac{8}{5}}\beta^{\frac{13}{5}}h^{\frac{6}{5}}|\log h|^K. \tag{28.4.14}$$

Remark 28.4.5. Observe that

(i) If assumption $(28.2.27)^*$ holds, then $Q_0 \lesssim \kappa^{\frac{1}{3}}\beta^{\frac{4}{3}}h^{-\frac{4}{3}} \lesssim \beta h^{-2}$, where the middle expression appears in (28.2.25). On the other hand, if $(28.2.27)^*$ fails, then the reverse inequalities hold. In the general case we assume that $\beta h^2 \ll 1$ to get a remainder estimate smaller than the main term.

(ii) Also $\nu \lesssim \beta$ provided $(28.2.27)^*$ holds; if $\kappa = 1$ then $\nu \lesssim \beta$ if and only if $(28.2.27)^*$ holds.

28.4.3 Endgame

Similarly to Theorem 28.3.21 we arrive to

Theorem 28.4.6. *Let $\beta h \gtrsim 1$, $\kappa \le \kappa^*$ and $(28.2.27)^*$ be fulfilled. Then estimate* (28.3.78)

$$|\mathsf{E}^*_\kappa - \mathcal{E}^*_\kappa| \le CQ$$

holds where

(i) Under non-degeneracy assumption (28.3.65) *Q is defined by* (28.4.12) *and* (28.4.13).

(ii) In the general case Q is defined by (28.4.12)*; in particular, $Q = \beta h^{-\frac{1}{2}}$ as $\kappa\beta h \lesssim 1$.*

Problem 28.4.7[20]. In this new settings recover estimates for $\|\partial(A' - A'')\|$, $\|\partial(A' - A'')\|_{\mathscr{L}^\infty}$ and $\|\partial A'\|_{\mathscr{L}^\infty}$ where A'' is a minimizer for $\bar{\mathcal{E}}(A'')$.

28.4.4 N-Term Asymptotics and D-Term Estimates

Repeating arguments of the proofs of Propositions 28.3.24, 28.3.26 we arrive to

Proposition 28.4.8. *Let $\beta h \gtrsim 1$ and conditions $(28.3.49)_{1,2}$ be fulfilled. Then*

(i) Under non-degeneracy assumption (28.3.60) *or* (28.3.63) *estimate* (28.3.84) *holds with $R = R_0 + R'$,*

$$R_0 = \beta h^{-1} + \beta h^{-\frac{2}{3}}\nu^{\frac{2}{3}} \tag{28.4.15}$$

and R' defined by $(28.3.61)'$.

[20] Cf. Problem 28.3.22.

(ii) Under non-degeneracy assumption (28.3.63) *estimate* (28.3.84) *holds with* $R = R_0 + R''$, R_0 *and* R'' *defined by* (28.4.15) *and* (28.3.86).

(iii) In the general case estimate (28.3.84) *holds with* $R = R_0 + R'''$, R_0 *and* R''' *defined by* (28.4.15) *and* (28.3.88).

Repeating arguments of the proof of Propositions 28.3.27 and 28.3.27 we arrive to

Proposition 28.4.9. *Let* $\beta h \gtrsim 1$ *and conditions* $(28.3.49)_{1,2}$ *be fulfilled. Then*

(i) Under non-degeneracy assumptions (28.3.60) *or* (28.3.63) D*-term* (28.3.89) *does not exceed* CR^2 *with* $R = R_0 + R'$, R_0 *and* R' *defined by* (28.4.15) *and* $(28.3.61)'$ *respectively.*

(ii) Under non-degeneracy assumption (28.3.65) D*-term* (28.3.89) *does not exceed* CR^2 *with* $R = R_0 + R''$, R_0 *and* R' *defined by* (28.4.15) *and* (28.3.86).

(iii) In the general case D*-term* (28.3.89) *does not exceed* CR^2 *with* $R = R_0 + R'''$, R_0 *and* R' *defined by* (28.4.15) *and* (28.3.88).

Problem 28.4.10. In the general case (without any non-degeneracy assumptions) for $\beta h \lesssim 1$ and for $\beta h \gtrsim 1$ improve the remainder estimates for both the trace term and N-term and estimates for D-term (so, make R''' and Q''' smaller) under assumption $V \in \mathscr{C}^s$ with $s > 2$.

To do this use more advanced partition of unity as in Chapter 25. Most likely, however, it will affect only terms $C\beta h^{-\frac{1}{2}}$ and $C\beta h^{-\frac{3}{2}}$ in Q''' and R''' replacing them by $C\beta h^{(s-4)/(s+2)}$ and $C\beta h^{-1-2/(s+2)}$ respectively.

28.5 Global Trace Asymptotics in the Case of Thomas-Fermi Potential: $B \le Z^{\frac{4}{3}}$

28.5.1 Introduction

In this Section we consider global trace asymptotics for Thomas-Fermi potential. First we consider the singularity zones where our results would follow from Section 27.3, then we consider their interaction with the regular zone which would lead to the deterioration of the remainder estimates for

$\beta \gg h^{-\frac{1}{2}}$ and finally the boundary zone where non-degeneration properties could be violated (especially for $M \geq 2$), which requires rather subtle analysis and usage of the specific properties of Thomas-Fermi potential.

Remark 28.5.1. Recall that according to Chapter 25 there are two cases:

(a) $B \leq Z^{\frac{4}{3}}$, when the most contributing to both the number of particles and the energy zone is $\{x\colon \ell(x) \asymp r^* = Z^{-\frac{1}{3}}\}$ (where $\ell(x)$ is the distance to the closest nucleus), and then rescaling $x \mapsto x r^{*\,-1}$, $\tau \mapsto \tau Z^{-\frac{4}{3}}$ we arrive in this zone to $\beta = BZ^{-1}$, $h = Z^{-\frac{1}{3}}$ with $\beta h \leq 1$.

(b) $Z^{\frac{4}{3}} \leq B \leq Z^3$, when the most contributing to both the number of particles and the energy zone is $\{x\colon \ell(x) \asymp r^* = B^{-\frac{2}{5}} Z^{\frac{1}{5}}\}$, and then rescaling $x \mapsto x r^{*\,-1}$, $\tau \mapsto \tau B^{-\frac{2}{5}} Z^{-\frac{4}{5}}$ we arrive in this zone to $\beta = B^{\frac{2}{5}} Z^{-\frac{1}{5}}$, $h = B^{\frac{1}{5}} Z^{-\frac{3}{5}}$ with $\beta h \geq 1$.

We also recall that in the free (movable) nuclei model the distances between nuclei were greater than ϵr^* (which would be the case in the current settings as well as we show later), so we will assume that it is the case deducting our main results.

28.5.2 Estimates to a Minimizer

Preliminary Analysis

Consider potential V with the Coulomb-like singularities, exactly as in Section 27.3 i.e. satisfying (27.3.1)–(27.3.3).

Proposition 28.5.2 [21]**.** *Let V satisfy* (27.3.1)–(27.3.2) *and*

$$|D^\alpha W| \leq C_\alpha \sum_{1\leq m\leq M} z_m \bigl(|x-\bar{y}_m|+1\bigr)^{-4} |x-\bar{y}_m|^{-|\alpha|} \qquad \forall \alpha : |\alpha| \leq 2. \tag{28.5.1}$$

Let $\kappa \leq \kappa^*$ and $\beta h \leq 1$. Then the near-minimizer A satisfies

$$|\operatorname{Tr}(H^-_{A,V}) + \int h^{-3} P_{\beta h}(V(x))\Bigr)\, dx| \leq Ch^{-2} \tag{28.5.2}$$

and

$$\|\partial A'\| \leq C\kappa^{\frac{1}{2}}. \tag{28.5.3}$$

[21] Cf. Proposition 27.3.1.

Proof. We follow the proof of Proposition 27.3.1. Observe that scaling $x \mapsto (x - \bar{y}_m)\ell^{-1}$, $\tau \mapsto \tau\zeta^{-2}$ leads us to

$$h \mapsto h_1 = h\ell^{-1}\zeta^{-1}, \qquad \beta \mapsto \beta_1 = \beta\ell\zeta^{-1}, \qquad \kappa \mapsto \kappa_1 = \kappa\zeta^2\ell. \tag{28.5.4}$$

Also observe that for $\zeta = \ell^{-\frac{1}{2}}$

$$\kappa_1\beta_1 h_1^2 \gtrsim 1 \implies \ell \gtrsim \ell^* = (\beta+1)^{-\frac{1}{2}}h^{-1} \tag{28.5.5}$$

and for $\kappa \asymp 1$ those are equivalent.

(i) First, we pick up $A' = 0$. Then

$$|\operatorname{Tr}\bigl(H^-_{A^0,V}(0)\bigr) + h^{-3}\int P_{\beta h}(V(x))\,dx| \le Ch^{-2}; \tag{28.5.6}$$

this estimate follows from the standard partition with ℓ-admissible partition elements, supported in $\{x\colon \ell(x) \lesssim \ell\}$ for $\ell = \ell_*$ and and in $\{x\colon \ell(x) \asymp \ell\}$ for $\ell \ge 2\ell_*$.

(ii) On the other hand, consider $A' \ne 0$. Let us prove first that

$$\operatorname{Tr}^-(\psi_\ell H\psi_\ell) \ge -C_\varepsilon h^{-2} - \varepsilon\kappa^{-1}h^{-2}\|\partial A'\|^2 \tag{28.5.7}$$

for $\ell = \ell_* = h^2$ where one can select constant ε arbitrarily small.

Rescaling $x \mapsto (x - \bar{y}_m)/\ell$ and $\tau \mapsto \tau/\ell$ and therefore $h \mapsto h\ell^{-\frac{1}{2}} \asymp 1$ and $A \mapsto A\ell^{\frac{1}{2}}$ (because singularity is Coulomb-like), we arrive to the same problem with the same κ and with $\ell = h = 1$ and with β replaced by βh^3. Then for $\beta h^3 \le 1$ we refer to Appendix 27.A.1 since $H_{A,V} \ge H_{A',V'}$ with $V' = V - \beta^2|x|^2$.

(iii) Consider now ψ_ℓ as in (i) with $\ell \ge \ell_*$. Then according to Theorems 28.3.21 and 28.4.6 for $\beta_1 h_1 \lesssim 1$ and $\kappa\zeta^2\ell \le \kappa^*$

$$\operatorname{Tr}^-\bigl(\psi_\ell H_{A,V}\psi_\ell\bigr) + h^{-3}\int P_{\beta h}(V(x))\psi_\ell^2(x)\,dx \\ \ge -C_\varepsilon\zeta^2(h_1^{-1} + \beta_1 h_1^{-1}) - \varepsilon\kappa^{-1}h^{-2}\|\partial A'\|^2. \tag{28.5.8}$$

Remark 28.5.3. Observe that if ψ_ℓ is supported in $\{x\colon \frac{1}{2}r \le \ell(x) \le 2r\}$, then we can take a norm of $\partial A'$ over $\{x\colon \frac{1}{4}r \le \ell(x) \le 4r\}$. Indeed, we can just replace A' by $A'' = \phi_\ell(A' - \eta)$ with arbitrary constant η and with ϕ_ℓ supported in $\{x\colon \frac{1}{4}r \le \ell(x) \le 4r\}$ and equal 1 in $\{x\colon \frac{1}{3}r \le \ell \le 3r\}$ (and ε by $c\varepsilon$).

Then summation of these norms returns $-C_0\varepsilon\kappa^{-1}h^{-2}\|\partial A'\|^2$.

Furthermore, the first term in the right-hand expression of (28.5.8) is $-C_\varepsilon(\zeta^3\ell^{-1}h^{-1}+\zeta^2\ell^2\beta h^{-1})$ and summation over $\ell\geq h^2$ returns $-C_\varepsilon h^{-2}$ since $\zeta=\min(\ell^{\frac{1}{2}},\,\ell^{-2})$.

(iv) Consider next zone where $\beta_1 h_1\geq 1$ (and $\ell\geq 1$) but still $h_1\leq 1$. According to previous Section 28.5 inequality (28.5.8) should be replaced by

$$\operatorname{Tr}^-\bigl(\psi_\ell H_{A,V}\psi_\ell\bigr)+h^{-3}\int P_{\beta h}(V(x))\psi_\ell^2(x)\,dx \geq -C_\varepsilon\zeta^2\beta_1 h_1^{-1}\bigl(1+\nu_1^{\frac{4}{3}}h_1^{\frac{5}{3}}\bigr)-\varepsilon\kappa^{-1}h^{-2}\|\partial A'\|^2 \tag{28.5.9}$$

with $\nu_1=(\kappa_1\beta_1)^{\frac{10}{9}}h_1^{\frac{4}{9}}|\log h|^K$ [22] and $\kappa_1\beta_1=\kappa\beta\zeta\ell^2=\kappa\beta$ and thus with $\beta_1 h_1^{-1}\zeta^2=\beta h^{-1}\zeta^2\ell^2$. Then summation of the first term in the right-hand expression results in its value when ℓ is the smallest i.e. $\beta_1 h_1=1$ and one can check easily[23] that this is less than Ch^{-2}.

Further, Remark 28.5.3 remains valid. Then adding this zone does not change inequality in question.

(v) The rest of the proof is obvious. Zone $\{x\colon \ell(x)\geq\ell^*\}$ is considered as a single element and just rough variational estimate is used there to prove that its contribution does not exceed Ch^{-2}. □

Remark 28.5.4. Later we will improve both upper and lower estimates using different tricks: imposing non-degeneracy assumptions, picking for an upper estimate semiclassical self-generated magnetic field, using Scott approximation terms. These improvements will lead not only to our final goal, but also to our intermediate one–getting better estimates for a minimizer.

Proposition 28.5.5 [24]**.** *In the framework of Proposition 28.5.2 there exists a minimizer A.*

Proof. After Proposition 28.5.2 has been proven we just repeat arguments of the proof of Proposition 27.2.2. □

[22] Because $\kappa_1\beta_1 h_1=\kappa\beta h\ell\leq\kappa(\beta h)^{\frac{3}{4}}\leq 1$.

[23] Sufficient to check for $\beta=h^{-1}$, $\ell=1$ and $\kappa=1$.

[24] Cf. Proposition 27.3.2.

Estimates to a Minimizer: Interior Zone

Recall equation (27.2.14) for a minimizer A:

$$\frac{2}{\kappa h^2}\Delta A_j(x) = \Phi_j := -\operatorname{Re}\operatorname{tr}\upsigma_j\Bigl((hD-A)_x\cdot\boldsymbol{\sigma} e(x,y,\tau)+e(x,y,\tau)\,{}^t(hD-A)_y\cdot\boldsymbol{\sigma}\Bigr)\Bigr|_{y=x}. \tag{27.2.14}$$

After rescaling $x\mapsto x/\ell$, $\tau\mapsto\tau/\zeta^2$, $h\mapsto\hbar=h/(\zeta\ell)$, $A\mapsto A\zeta^{-1}\ell$, $\beta\mapsto\beta\zeta^{-1}\ell$ this equation becomes (27.3.13)

$$\Delta A_j = -2\kappa\zeta^2\ell\hbar^2\operatorname{Re}\operatorname{tr}\upsigma_j\Bigl((\hbar D-\zeta^{-1}A)_x\cdot\boldsymbol{\sigma} e(x,y,\tau)+e(x,y,\tau)\,{}^t(\hbar D-\zeta^{-1}A)_y\cdot\boldsymbol{\sigma}\Bigr)\Bigr|_{y=x} \tag{27.3.13}$$

and since we can take $\zeta^2\ell=1$ we arrive to (27.3.14)

$$\Delta A_j = -2\kappa\hbar^2\operatorname{Re}\operatorname{tr}\upsigma_j\Bigl((\hbar D-\zeta^{-1}A)_x\cdot\boldsymbol{\sigma} e(x,y,\tau)+e(x,y,\tau)\,{}^t(\hbar D-\zeta^{-1}A)_y\cdot\boldsymbol{\sigma}\Bigr)\Bigr|_{y=x}. \tag{27.3.14}$$

Let us modify arguments of Subsection 27.3.1. First observe that

$$|\partial A'|\le C\kappa^{\frac{1}{2}}h^{-3},\quad |\partial^2 A'|\le C\kappa^{\frac{1}{2}}h^{-5}\qquad\text{for}\quad \ell\le 2\ell_* \tag{28.5.10}$$

with $\ell_*=h^2$; this follows from above equations rescaled and from $\beta h^3\le\epsilon_0$. Let

$$\mu(r)=\sup_{\ell(x)\ge r}|\partial A'|\ell\zeta^{-1},\qquad \nu(r)=\sup_{\ell(x)\ge r}|\partial^2 A'|\ell^2\zeta^{-1}; \tag{28.5.11}$$

then $\nu(r)$ should not exceed[25)]

$$\begin{aligned}F(\nu)=C\kappa_1\Bigl(1+\mu+\min\bigl(\beta_1^{\frac{3}{2}}h_1^{\frac{1}{2}},\,\beta_1^{\frac{1}{2}}\bigr)\\ +\beta_1 h_1\bigl(\nu^{\frac{1}{10}}h_1^{-\frac{3}{5}}+\nu^{\frac{1}{7}}h_1^{-\frac{4}{7}}+\nu^{\frac{1}{4}}h_1^{-\frac{1}{2}}|\log h_1|^2\bigr)\Bigr)|\log h_1|+C\kappa^{\frac{1}{2}}(\ell\zeta^2)^{-\frac{1}{2}},\end{aligned} \tag{28.5.12}$$

where here $\nu=\nu(\frac{1}{2}r)$, $\mu=\mu(r)$, the last term is just an estimate for $\|\partial A'\|$ rescaled and $\ell\asymp r$ in that term. Indeed, (28.5.12) is derived exactly as (28.3.46), but here we cut a hole $\{x\colon \ell(x)\le\frac{1}{2}r\}$ in our domain.

25) As long as $\beta_1 h_1\le 1$.

We also know that $\mu \le C\nu^{\frac{3}{5}}\kappa^{\frac{1}{5}}(\ell\zeta^2)^{-\frac{1}{5}}$. Using (28.5.12) and (28.5.10) one can prove easily that $\nu(r)$ does not exceed solution of the equation $\nu = F(\nu)$ multiplied by C[26], i.e.

$$\nu \le C\kappa_1\Bigl(1 + \min\bigl(\beta_1^{\frac{3}{2}} h_1^{\frac{1}{2}},\, \beta_1^{\frac{1}{2}}\bigr)\Bigr)|\log h_1| + C\Bigl((\kappa_1\beta_1)^{\frac{10}{9}} h_1^{\frac{4}{9}} + (\kappa_1\beta_1)^{\frac{4}{3}} h_1^{\frac{2}{3}}\Bigr)|\log h_1|^K + C\kappa^{\frac{1}{2}}(\ell\zeta^2)^{-\frac{1}{2}}. \tag{28.5.13}$$

In particular, scaling back and setting $\zeta = \ell^{-\frac{1}{2}}$ we arrive to

$$|\partial^2 A'| \le C\kappa\Bigl(\ell^{-\frac{5}{2}} + \min\bigl(\beta^{\frac{3}{2}} h^{\frac{1}{2}}\ell^{-\frac{1}{2}},\, \beta^{\frac{1}{2}}\ell^{-\frac{7}{4}}\bigr)\Bigr)|\log \ell/\ell_*| + C\Bigl((\kappa\beta)^{\frac{10}{9}} h^{\frac{4}{9}}\ell^{-\frac{19}{18}} + (\kappa\beta)^{\frac{4}{3}} h^{\frac{2}{3}}\ell^{-\frac{5}{6}}\Bigr)|\log \ell/\ell_*|^K + C\kappa^{\frac{1}{2}}\ell^{-\frac{5}{2}}. \tag{28.5.14}$$

The same arguments work for $\beta_1 h_1 \ge 1$ but now we need to replace $|\log h_1|$ by $|\log \beta_1|$ which however is also $\asymp \ell/\ell_*$ as $\beta h \le 1$.

After this estimate is proven we can remove the last term in the right-hand expression and we arrive to

Proposition 28.5.6. *In the framework of Proposition 28.5.2*

$$|\partial^2 A'| \le C\kappa\Bigl(\ell^{-\frac{5}{2}} + \min\bigl(\beta^{\frac{3}{2}} h^{\frac{1}{2}}\ell^{-\frac{1}{2}},\, \beta^{\frac{1}{2}}\ell^{-\frac{7}{4}}\bigr)\Bigr)|\log \ell/\ell_*| + C\Bigl((\kappa\beta)^{\frac{10}{9}} h^{\frac{4}{9}}\ell^{-\frac{19}{18}} + (\kappa\beta)^{\frac{4}{3}} h^{\frac{2}{3}}\ell^{-\frac{5}{6}}\Bigr)|\log \ell/\ell_*|^K. \tag{28.5.15}$$

Estimates to a Minimizer: Exterior Zone

Let us estimate $|\partial^2 A'|$ as $\ell \ge \ell^*$. Observe that

$$A'_j(x) = -\frac{\kappa h^2}{4\pi}\int |x-y|^{-1}\Phi_j(y)\,dy, \tag{28.5.16}$$

where Φ_j is given by (27.2.14). Then $\partial^2 A'$ is expressed via Φ_j as an integral with a kernel $K(x,y)$, singular when $x = y$ and such that $|K(x,y)| \le c(|x|+|y|)^{-3}$ when $|x-y| \asymp |x|+|y|$. Further, applying representation like in Proposition 27.3.9, we can get an extra factor $|y|(|x|+|y|)^{-1}$ upgrading it to $|K(x,y)| \le c|y|(|x|+|y|)^{-4}$.

[26] As long as a resulting expression rescaled, see (28.5.14) is a decaying function of ℓ.

Then, starting from (28.5.15) and iterating (28.3.46) we arrive to estimate

$$|\partial^2 A'| \le C\kappa \ell^{-4}|\log h| + C(\kappa\beta)^{\frac{10}{9}} h^{\frac{4}{9}}\ell^{-\frac{32}{9}+\delta}|\log h|^K \qquad \text{for } \ \ell\ge 1$$

with arbitrarily small $\delta > 0$. Furthermore, using arguments of the proof of Proposition 28.5.6 we can make $\delta = 0$ thus arriving to

Proposition 28.5.7. *In the framework of Proposition 28.5.2*

$$|\partial^2 A'| \le C\kappa \ell^{-4}|\log h| + C(\kappa\beta)^{\frac{10}{9}} h^{\frac{4}{9}}\ell^{-\frac{32}{9}}|\log h|^K \qquad \textit{for } \ \ell\ge 1. \tag{28.5.17}$$

Remark 28.5.8. Sure, as $\ell \ge 1$, $\beta_1 h_1^{\frac{1}{2}}|\log h_1|^K \le 1$ this estimate could be improved but these improvements would not affect our crucial estimates.

28.5.3 Trace Asymptotics

Before proving trace estimates observe

Remark 28.5.9. (i) All local asymptotics and estimates with with mollification with respect to spatial variables [27] proven in Sections 28.3 and 28.4 with unspecified $\nu \le \epsilon\beta$ remain valid in the more general framework of the smooth non-degenerate external field $A^0(x)$: namely

$$\|\partial^4 A^0\| \le C_0\beta, \qquad B^0 = |\nabla \times A^0| \ge \epsilon_0\beta. \tag{28.5.18$_{1,2}$}$$

Indeed, we use only ε-approximations with $\varepsilon = h$ or $\varepsilon = h\rho^{-1}$ and we can always change coordinate system so magnetic lines are $(x_1, x_2) = \mathsf{const}$. We leave easy arguments to the reader.

(ii) However since we do not have estimates (28.3.47) or (28.4.7)–(28.4.9) in this more general framework[28], we also do not have (28.4.12), (28.4.13) then.

Now consider the trace term assuming that

$$d := \min_{1\le m<m'\le M} |\bar{y}_m - \bar{y}_{m'}| \gtrsim 1. \tag{28.5.19}$$

[27] Thus trace and N-term asymptotics and D-term estimates.

[28] Even if we believe that these estimates are true. So far we have no need in such generalization.

(a) Due to the proofs of Theorem 27.3.22 and Proposition 28.5.2 we can evaluate contribution of the zone $\{x\colon |x-\bar{y}_m|\le\epsilon\}$, provided $\beta\le 1$:

$$\begin{aligned} &|\operatorname{Tr}(H^-_{A,V}\psi_m)-\operatorname{Tr}(H^-_{A,V_m}\psi_m)\\ &+h^{-3}\int P_{Bh}(V)\psi_m\,dx-h^{-3}\int P_0(V_m)\psi_m\,dx|\le C\bigl(h^{-1}+\kappa|\log\kappa|^{\frac{1}{3}}h^{-\frac{4}{3}}\bigr),\end{aligned}\tag{28.5.20}$$

where $V_m=z_m|x-\bar{y}_m|^{-1}$ and ψ_m is supported in $\{x:|x-\bar{y}_m|\le\epsilon\}$ and equal 1 in $\{x:|x-\bar{y}_m|\le\frac{1}{2}\epsilon\}$.

Further, we can replace in this estimate $\operatorname{Tr}(H^-_{A',V_m}\psi_m)+h^{-3}\int P_0(V_m)\psi_m$ by

$$\int\Bigl(\int_{-\infty}^0 e_{V_m,A'}(x,x,\tau)\,d\tau+h^{-3}P_0(V_m)\Bigr)\psi_m\,dx\tag{28.5.21}$$

and we can also replace in the latter expression ψ_m by 1.

(b) If $\beta\ge 1$, we can apply estimate (28.5.20) to the zone $\{x\colon|x-\bar{y}_m|\le\epsilon b\}$ with $b=\beta^{-\frac{2}{3}}$ scaling $x\mapsto(x-\bar{y}_m)b^{-1}$ and $\tau\to\tau$ and $h\mapsto h_1=hb^{-\frac{1}{2}}$, $\beta\mapsto\beta b^{\frac{3}{2}}=1$, $\kappa\mapsto\kappa$; now ψ_m is supported in $\{x:|x-\bar{y}_m|\le\epsilon b\}$ and equals 1 in $\{x:|x-\bar{y}_m|\le\frac{1}{2}\epsilon b\}$ and the right-hand expression of (28.5.20) becomes

$$Cb^{-1}\bigl(h_1^{-1}+\kappa|\log\kappa|^{\frac{1}{3}}h_1^{-\frac{4}{3}}\bigr)=C\bigl(\beta^{\frac{1}{3}}h^{-1}+\kappa|\log\kappa|^{\frac{1}{3}}\beta^{\frac{2}{9}}h^{-\frac{4}{3}}\bigr).\tag{28.5.22}$$

If $\beta\ge1$, let us consider contribution of the zone $\{x\colon\epsilon_0 b\le|x-\bar{y}_m|\le\epsilon_0\}$, where due to assumption (28.5.19) non-degeneracy condition (28.3.60) is automatically satisfied after rescaling; namely before rescaling it is

$$\min_j|V-2j\beta h|+|\nabla V|\ell\asymp\zeta^2.\tag{28.5.23}$$

A contribution of ℓ-element in this zone does not exceed

$$C\zeta^2\bigl(h_1^{-1}+h_1^{-\frac{1}{3}}\nu^{\frac{4}{3}}\bigr)\tag{28.5.24}$$

with

$$\nu=\sup_{|x-\bar{y}_m|\asymp\ell}|\partial^2A'|\ell^2\zeta^{-1},\tag{28.5.25}$$

and plugging (28.5.4) into (28.5.24) we get

$$C\bigl(\ell^{-\frac{1}{2}}h^{-1}+(\kappa\beta)^{\frac{40}{27}}h^{\frac{7}{27}}\ell^{\frac{59}{54}}|\log(h\ell^{-\frac{1}{2}})|^K\bigr),$$

which sums to

$$C\bigl(\beta^{\frac{1}{3}}h^{-1}+(\kappa\beta)^{\frac{40}{27}}h^{\frac{7}{27}}|\log h|^{K}\bigr), \tag{28.5.26}$$

which obviously does not exceed (28.5.22). Thus after scaling[29)] we arrive to

Proposition 28.5.10. *Let $V=W_B^{\mathsf{TF}}+\lambda$ be Thomas-Fermi potential with $N\le Z$, $N\asymp Z_1\asymp Z_2\asymp ...\asymp Z_M$, $B\lesssim Z^{\frac{4}{3}}$ and*

$$|\mathsf{y}_m-\mathsf{y}_{m'}|\ge d\gtrsim Z^{-\frac{1}{3}}\qquad \forall 1\le m<m'\le M. \tag{28.5.27}$$

Then if ψ_m is supported in ϵr^*-vicinity of y_m

$$\begin{gathered}|\operatorname{Tr}(H^-_{A,V}\psi_m)-\operatorname{Tr}(H^-_{A,V_m}\psi_m)\\ +\int P_B(V)\psi_m\,dx-\int P_0(V_m)\psi_m\,dx|\end{gathered} \tag{28.5.28}$$

does not exceed CQ_0 with

$$Q_0:=\left\{\begin{aligned}&\bigl(Z^{\frac{5}{3}}+\alpha|\log(\alpha Z)|^{\frac{1}{3}}Z^{\frac{25}{9}}\bigr) &&\textit{for}\quad B\le Z,\\ &\bigl(B^{\frac{1}{3}}Z^{\frac{4}{3}}+\alpha|\log(\alpha Z)|^{\frac{1}{3}}B^{\frac{2}{9}}Z^{\frac{23}{9}}\bigr) &&\textit{for}\quad Z\le B\le Z^{\frac{4}{3}}.\end{aligned}\right. \tag{28.5.29}$$

Furthermore, if $B\le Z$, then expression (28.5.28) *does not exceed*

$$C\Bigl(Z^{\frac{5}{3}}[Z^{-\delta}+(BZ^{-1})^{\delta}+(dZ^{\frac{1}{3}})^{-\delta}]+\alpha|\log(\alpha Z)|^{\frac{1}{3}}Z^{\frac{25}{9}}\Bigr). \tag{28.5.30}$$

Here improved estimate (28.5.30) can be proven by our standard propagation arguments.

Further, let us consider the *regular exterior zone* $\{x\colon \epsilon_0 r^*\le |x-\mathsf{y}_m|\le \epsilon\bar{r}\}$ with $\bar{r}:=\min\bigl(B^{-\frac{1}{4}},\,(Z-N)_+^{-\frac{1}{3}}\bigr)$. Then due to Thomas-Fermi equation $W_B^{\mathsf{TF}}+\lambda$ satisfies here non-degeneracy condition (28.3.65) after rescaling and $\zeta=\ell^{-2}$, $h_1=\ell(x)$, $\beta_1=B\ell^3$.

Then the contribution of ℓ-element in this zone does not exceed (28.5.25) as long as $\beta_1h_1\le 1$, $h_1\le 1$ i.e. $\ell(x)\le\min(\bar{r},1)$, and due to (28.5.24) this contribution does not exceed $C\zeta^2\bigl(h_1^{-1}+h_1^{-\frac{1}{3}}\nu^{\frac{4}{3}}\bigr)$, where ν_1 is estimate for $|\partial^2A'|$ multiplied by $\zeta^{-1}\ell^2$:

$$\nu_1=\kappa|\log h|+(\kappa\beta)^{\frac{10}{9}}h^{\frac{4}{9}}\ell^{\frac{4}{9}}|\log h|^{K}. \tag{28.5.31}$$

29) $x\mapsto Z^{\frac{1}{3}}x$, $\tau\mapsto Z^{\frac{4}{3}}\tau$, $1\mapsto h=Z^{-\frac{1}{3}}$, $B\mapsto\beta=Z^{-1}$, $\alpha\mapsto\kappa=\alpha Z$; recall that $\beta h\lesssim 1\iff B\lesssim Z^{-\frac{4}{3}}$.

Then calculating ν_1 and plugging it and $h_1 = h\ell$ into $C\zeta^2\bigl(h_1^{-1} + h_1^{-\frac{1}{3}}\nu^{\frac{4}{3}}\bigr)$ one can see easily that here all terms contain ℓ in the negative powers.

Then summation by ℓ results in the same expression calculated for $\ell = r^*$ and one can observe easily that it does not exceed (28.5.29), (28.5.30) for $B \le Z$, $Z \le B \le Z^{\frac{4}{3}}$ respectively. One can see easily that dealing with terms $C\zeta^2 \times \mu^3\beta^{-2}h^{-2}$ due to (28.3.61) and $C\zeta^2\nu|\log h|$ (see Propositions 28.3.13 and 28.3.15) leads to smaller expressions.

Furthermore, using the standard propagation arguments one can upgrade (28.5.29) to (28.5.30). Therefore we conclude that

(28.5.32) Proposition 28.5.10 remains true for ψ_m supported in the zone $\{x\colon |x - \mathsf{y}_m| \le \epsilon \min(\bar{r}, 1)\}$.

Consider now the contribution of the *boundary zone* $\{x\colon \ell(x) \ge \min(\bar{r}, 1)\}$.

(a) Let us start from more difficult and interesting case $B \ge 1$ assuming first that $Z = N$. Rescale this zone first $x \mapsto xB^{\frac{1}{4}}$, $\tau \mapsto \tau B^{-1}$, then we have $h_1 = B^{-\frac{1}{4}}$, $\beta_1 = B^{\frac{1}{4}}$. Observe that

(28.5.33) After this rescaling a rescaled magnetic field satisfies $|\partial^2 A'| \le \nu_1$ where ν_1 is given by (28.5.31) for $\ell = \bar{r}$.

As we know from Subsection 26.5.1, after the first scaling there exists the scaling function γ such that

$$|\partial^\alpha V| \le C\gamma^{4-|\alpha|} \qquad |\alpha| \le 4, \tag{28.5.34}$$

$$V \asymp \gamma^4, \qquad |\partial^2 V| \asymp \gamma^2 \tag{28.5.35}$$

and therefore we can use a γ-admissible partition. Then scaling again $x \mapsto x\gamma^{-1}$, $\tau \mapsto \tau\gamma^{-4}$, $h_1 \mapsto h_2 = h\gamma^{-3}$, $\beta_1 \mapsto \beta_2 = \beta_1\gamma^{-1}$ and $\nu_1 \mapsto \nu_2 = \nu_1$ we see that non-degeneracy assumption (28.3.65) is fulfilled and therefore according to Proposition 28.4.3(ii) the contribution of γ-element to the remainder does not exceed $CB\gamma^4\beta_2\bigl(1 + h_2^{\frac{2}{3}}\nu_2^{\frac{4}{3}}\bigr)$ because now $\beta_2 h_2 \ge 1$. Then the total contribution of such elements does not exceed

$$CB\int \beta_2\bigl(1 + h_2^{\frac{2}{3}}\nu_2^{\frac{4}{3}}\bigr)\gamma^{-3}\,dx \tag{28.5.36}$$

with integral taken over zone $\{x\colon \gamma(x)\ge \bar\gamma := h_1^{\frac{1}{3}}\}$ where $h_2\le 1$. Plugging β_2, h_2 and $\nu_2=\nu_1$ we get in the second term γ^{-2} which is not good. Let us apply Remark 28.5.9.

Recall that $A'(x)$ is a solution of the Laplace equation and therefore $A'(x)=\int |x-y|^{-1}F(y)\,dy$; then $A'(x)$ with $x\in B(z,\gamma(z))$ can be decomposed into the sum of two terms; the first one is given by the integral over $\{y : |y-z|\ge \frac{3}{2}\gamma(z)\}$ and therefore is smooth and could be included in $A^0(x)$ while the second is given by integral over $\{y : |y-z|\le 2\gamma(z)\}$ and could be estimated by (28.3.46) with β, h, κ and ν replaced by β_2, h_2, $\kappa_2=\kappa_1\gamma^5$ and ν_1 and then one can see easily that $\nu_2\le \nu_1\gamma^{\frac{3}{2}+\delta}$. Therefore we conclude that

Remark 28.5.11. In the boundary zone calculating trace term, N- and D-terms one can take $\nu_2=\nu_1\gamma^{\frac{3}{2}+\delta}$ with $\delta>0$.

Plugging this improved ν_2 into (28.5.36) we get everywhere γ in the positive power and therefore expression (28.5.36) does not exceed the integrand for $\gamma=1$, which is $CB\beta_1\bigl(1+h_1^{\frac{2}{3}}\nu_1^{\frac{4}{3}}\bigr)$, which we already got when estimating the contribution of the regular zone.

(b) In the zone $\{x\colon \gamma(x)\le\bar\gamma\}$ we just reset $\gamma=\bar\gamma$ and since $h_2\asymp 1$ we do not need any non-degeneracy condition here. Thus its contribution does not exceed $CB\beta_1$. Therefore we arrive to Proposition 28.5.12(i) with $Z=N$ and $B\ge 1$.

(c) In the case $B\le 1$ we need no non-degeneracy assumption in the zone $\{x\colon \ell(x)\gtrsim 1\}$ as $h_1=1$; Proposition 28.5.12(i) has been proven in this case as well.

(d) Explore now case $N<Z$. Then eventually we will need to take $V=W_B^{\mathsf{TF}}+\lambda$, where λ is a chemical potential. In this case the same arguments hold provided $B\gamma^4\le|\lambda| \implies \gamma\le h_1^{\frac{1}{3}}$ which is equivalent to $(Z-N)_+\le B^{\frac{5}{12}}$ since in this case $-\lambda\asymp (Z-N)_+\bar r^{-1}=(Z-N)_+B^{\frac{1}{4}}$.

(e) Further, for $M=1$ we do not need assumption $N=Z$ since we can always refer to non-degeneracy condition (28.5.23), which is fulfilled, and we arrive to Proposition 28.5.12(ii). Indeed, as in Section 26.5 we do not partition further elements where this condition is fulfilled. We arrive to Proposition 28.5.12(i), (ii) below.

(f) Furthermore, consider case $M\geq 2$ and $B^{\frac{5}{12}}\leq (Z-N)_+\leq B^{\frac{3}{4}}$. Then $B\bar{\gamma}^4=(Z-N)_+B^{\frac{1}{4}}$ and $\bar{\gamma}=(Z-N)_+^{\frac{1}{4}}B^{-\frac{3}{16}}$.

In this case the contribution of $\bar{\gamma}$-element (in the excess what was prescribed before) does not exceed term (28.3.66) multiplied by ζ^2. Note that two last terms in (28.3.66) are not new. Meanwhile, the first term there (i.e. $C\beta\nu^{\frac{6}{5}}h^{\frac{2}{5}}$) becomes $CB\bar{\gamma}^4\times B^{\frac{1}{4}}\bar{\gamma}^{-1}\times\bar{\nu}^{\frac{6}{5}}\times(B^{-\frac{1}{4}}\bar{\gamma}^{-3})^{\frac{2}{5}}$ and after multiplication by $\bar{\gamma}^{-2}|\log\bar{\gamma}|$ it has $\bar{\gamma}$ in the negative degree, so it does not exceed the same value for $\bar{\gamma}=B^{-\frac{1}{12}}$. After easy but tedious calculations one can see that it is less than (28.5.22).

This leaves us with the second term in (28.3.66) (i.e. $C\beta h^{-\frac{1}{2}}$), which becomes $CB\bar{\gamma}^4\times B^{\frac{1}{4}}\bar{\gamma}^{-1}\times B^{\frac{1}{8}}\bar{\gamma}^{\frac{3}{2}}$ and after multiplication by $\bar{\gamma}^{-2}|\log\bar{\gamma}|$ we get

$$CB^{\frac{11}{8}}\bar{\gamma}^{\frac{5}{2}}|\log\bar{\gamma}|\asymp CQ':=CB^{\frac{29}{32}}(Z-N)_+^{\frac{5}{8}}\bigl(1+|\log(Z-N)_+B^{-\frac{3}{4}}|\bigr). \tag{28.5.37}$$

(g) Finally, if $(Z-N)_+\geq B^{\frac{3}{4}}$, we again end up with the term $C\zeta^2\beta h^{-\frac{1}{2}}$ this time with $\zeta^2=(Z-N)_+^{\frac{4}{3}}$, $h=(Z-N)_+^{-\frac{1}{3}}$, $\beta=B(Z-N)_+^{-1}$ (now $\bar{\gamma}\asymp 1$); so we arrive to

$$CQ'':=CB(Z-N)_+^{\frac{1}{2}}. \tag{28.5.38}$$

Thus we arrive to Proposition 28.5.12(iii), (iv) below.

Proposition 28.5.12. *Let $V=W_B^{\mathsf{TF}}+\lambda$ be Thomas-Fermi potential with $N\leq Z$, $N\asymp Z_1\asymp Z_2\asymp\ldots\asymp Z_M$, $B\lesssim Z^{\frac{4}{3}}$ and chemical potential λ. Let assumption* (28.5.27) *be fulfilled. Then*

(i) For $Z=N$ ($\lambda=0$) the trace remainder

$$|\operatorname{Tr}(H_{A,V}^-)+\int P_{Bh}(V)\,dx-\sum_{1\leq m\leq M}\Bigl(\operatorname{Tr}(H_{A,V_m}^-\psi_m)-\int P_0(V_m)\psi_m\,dx\Bigr)| \tag{28.5.39}$$

does not exceed CQ_0 with Q_0 defined by (28.5.29)*; the same is true for $(Z-N)_+\leq B^{\frac{5}{12}}$.*

(ii) For $M=1$ *the trace remainder* (28.5.39) *also does not exceed* CQ_0.

(iii) For $M\ge 1$ *and* $B^{\frac{5}{12}}\le (Z-N)_+\le B^{\frac{3}{4}}$ *the trace remainder* (28.5.39) *does not exceed* $C(Q_0+Q')$ *with* Q' *defined by* (28.5.37).

(iv) For $M\ge 1$ *and* $(Z-N)_+^{\frac{4}{3}}\ge B$ *the trace remainder* (28.5.39) *does not exceed* $C(Q_0+Q'')$ *with* Q'' *defined by* (28.5.38).

Remark 28.5.13. (i) For $B\le Z$ expression (28.5.29) could be upgraded to (28.5.30).

(ii) Terms (28.5.38) and (28.5.39) are rather superficial: they do not depend on α and they were not present in Chapter 25. Indeed, using more precise arguments of Chapter 25 one can get rid of them, at least for sufficiently small α.

However in the upper estimate we will need to deal with D-term as well and this would give us a far larger error.

28.5.4 Endgame

Main Theorem: $M=1$

For $M=1$ we almost immediately arrive to the following statement which we formulate in "rescaled" terms:

Theorem 28.5.14. *Let* $V=W_B^{\mathsf{TF}}+\lambda$ *be a Thomas-Fermi potential as* $B\le Z^{\frac{4}{3}}$, $N\asymp Z$ *and* $M=1$. *Then*

$$\mathcal{E}_0^*+2S(\alpha Z)Z^2-CZ^{\frac{5}{3}}\bigl(1+\alpha B\bigr)\le \mathsf{E}_\alpha^* \le \mathcal{E}_\alpha^*+2S(\alpha Z)Z^2+C\bigl(Z^{\frac{5}{3}}+\alpha B^2 Z^{\frac{1}{3}}\bigr), \tag{28.5.40}$$

where $S(\alpha Z)Z^2$ *is a Scott correction term derived in Section 27.3.*

Proof: Estimate from above. We already know from (28.5.20) that after the standard rescaling for any magnetic field A' satisfying the same estimates as a minimizer of $\mathsf{E}_\kappa(A')$ the following estimate holds:

$$\operatorname{Tr}(H_{A,V}^-)+\kappa^{-1}h^{-2}\|\partial A'\|^2 \le -h^{-3}\int P_{Bh}(V)\,dx+\underbrace{(28.5.21)+\kappa^{-1}h^{-2}\|\partial A'\|^2}+(28.5.22). \tag{28.5.41}$$

Here the left-hand expression is $\mathsf{E}_\kappa(A') \ge \mathsf{E}^*_\kappa$ and in expression (28.5.21) we take $\psi_1 = 1$.

Let us pick up A' which is a minimizer for the Coulomb potential $V_1(x) = z_1|x - y_1|^{-1}$ without any external magnetic field[30]. Then we can replace the selected sum of two terms by $2h^{-2}S(\kappa z)z^2$ (in virtue of Subsubsection 27.3.5.1 an error does not exceed (28.5.22)).

Unfortunately A' is not a minimizer for a local problem; however we can replace $P_{Bh}(V)$ by

$$P_{\beta h}(V) + \partial_\beta P_{\beta h}(V)\cdot\Phi, \qquad \Phi = \partial_1 A'_2 - \partial_2 A'_1 \tag{28.5.42}$$

and, if we apply partition, then on each partition element an error in (28.5.41) does not exceed $C\kappa_1\zeta^2\beta_1 h_1^{-\frac{1}{2}} = C\kappa\beta h^{-\frac{1}{2}}\zeta^{\frac{5}{2}}\ell^{\frac{5}{2}}$. Indeed, we know that for a minimizer $\|\partial A'\| \le C(\kappa + \kappa^{\frac{1}{2}}h^{\frac{1}{2}})$ (also see in the proof of the estimate from below).

Summation over partition results in $C\kappa\beta^2$ and we arrive to

$$-h^{-3}\int P_{\beta h}(V)\,dx - h^{-3}\int \partial_\beta P_{\beta h}(V)\cdot\Phi\,dx + C(h^{-1} + \kappa\beta^2) \tag{28.5.43}$$

in the right-hand expression where the first term is $\mathcal{E}^*_0$[31].

The second term is rather unpleasant because we cannot estimate it by anything better than $C\beta h^{-1}$ (see in the estimate from below) but *here* we have a trick[32]: we replace A' by $-A'$ which is also a minimizer for the same Coulomb potential V_1 without external magnetic field. Then Φ and the second term change signs and since nothing else happens we can skip the second term which concludes the proof of the upper estimate.

Scaling back we arrive to the upper estimate in (28.5.40). □

Proof: Estimate from below. Again from (28.5.20) we already know that for a minimizer A' of $\mathsf{E}_\kappa(A')$ estimate (28.5.41) could be reversed

$$\begin{aligned}\operatorname{Tr}(H^-_{A,V}) &+ \kappa^{-1}h^{-2}\|\partial A'\|^2 \\ &\ge -h^{-3}\int P_{Bh}(V)\,dx + \underbrace{(28.5.21) + \kappa^{-1}h^{-2}\|\partial A'\|^2}\, - (28.5.22).\end{aligned} \tag{28.5.44}$$

[30] Actually since for the Coulomb potential the trace is infinite we take potential $V_1(x) + \tau$ with $\tau < 0$, establish estimates and then tend $\tau \to -0$.

[31] I.e. Thomas-Fermi energy calculated for $A' = 0$.

[32] Which unfortunately we cannot repeat in estimate from below.

Here the left-hand expression is $\mathsf{E}_\kappa(A') = \mathsf{E}^*_\kappa$ and the selected sum of two terms can be estimated from below by $2h^{-2}S(\kappa z)z^2$.

Again A' is not a minimizer for a local problem; however we can replace $P_{Bh}(V)$ by $P_{\beta h}(V)$ with an error not exceeding

$$Ch^{-3}\int |\partial_\beta P_{\beta h}(V)|\cdot|\partial A'|\,dx + Ch^{-3}\int |\partial^2_\beta P_{\beta h}(V)|\cdot|\partial A'|^2\,dx \\ \le Ch^{-3}\|\partial_\beta P_{\beta h}(V)\|\cdot\|\partial A'\| + Ch^{-3}\int |\partial^2_\beta P_{\beta h}(V)|\,dx \times \|\partial A'\|^2$$

with the right-hand expression not exceeding

$$C\beta h^{-1}|\partial A'\| + Ch^{-1}\|\partial A'\|^2. \tag{28.5.45}$$

However we already know that $\mathsf{E}^*_{2\kappa} \ge \mathcal{E}^*_0 - C(\kappa h^{-2} + h^{-1})$ and therefore since $\mathsf{E}_\kappa(A') = \mathsf{E}_{2\kappa}(A') + (2\kappa h^2)^{-1}\|\partial A'\|^2$ we conclude that

$$\|\partial A'\| \le C(\kappa + \kappa^{\frac{1}{2}}h^{\frac{1}{2}}); \tag{28.5.46}$$

then expression (28.5.45) does not exceed $C(\kappa\beta + 1)h^{-1}$ which concludes the proof of the lower estimate.

Since A' is a minimizer in the presence of the external field, we cannot replace A' by $-A'$ and thus cannot repeat the trick used in the proof of the upper estimate. Thus in the estimate from below we are left with $C\kappa\beta h^{-1}$ rather than with $C\kappa\beta^2$.

Scaling back we arrive to the lower estimate in (28.5.40). □

Remark 28.5.15. (i) It is a very disheartening that our estimate deteriorated here. However it may be that indeed the better estimate does not hold due to the *entanglement* of the singularity and the regular zone via self-generated magnetic field. Still we did not loose Scott correction term as long as $\kappa\beta h \ll 1$.

(ii) Recall that in the Section 27.3 we already had an entanglement of different singularities which obviously remains with us for $M \ge 2$. Surely both of these entanglements matter only if we are looking for the remainder estimate better than $O(\kappa h^{-2})$. Otherwise we can just pick up $A' = 0$ near singularities and the Scott correction term equal to $2h^{-2}S(0)z^2$;

(iii) The silver lining is that we do not need all these non-degeneracy conditions for such bad estimate and we expect that our arguments would work for $M\ge 2$. Still for $M\ge 2$ we will need to decouple singularities and to do this we will need to estimate $\|\partial A'\|_{\mathscr{L}^2(\{\ell(x)\asymp d\})}$ where d is the minimal distance between nuclei (see (28.5.19)).

For $\beta\ll 1$, $\kappa\ll h^{\frac{1}{3}}|\log h|^{-\frac{1}{3}}$ we can recover even Schwinger correction term:

Theorem 28.5.16. *Let V be a Thomas-Fermi potential $W_B^{\mathsf{TF}}+\lambda$ rescaled as $B\ll Z$, $N\asymp Z$ and $M=1$. Let respectively $\beta = BZ^{-1}$, $h=Z^{-\frac{1}{3}}$, and $\kappa=\alpha Z\le \kappa^*$. Then*

$$|\mathsf{E}^*_\alpha - \bigl(\mathcal{E}^*_0 + 2S(\alpha Z)Z^2 + \mathsf{Schwinger}\bigr)| \le CZ^{\frac{5}{3}}\bigl(Z^{-\delta}+B^\delta Z^{-\delta}\bigr) + C\alpha|\log \alpha Z|^{\frac{1}{3}}Z^{\frac{25}{9}} \tag{28.5.47}$$

where $\mathsf{Schwinger}$ *is a Schwinger correction term.*

Proof. The proof is standard like in Section 27.3: we invoke propagation arguments in the zone $\{x\colon (\beta+h)^\sigma \le \ell(x)Z^{\frac{1}{3}}\le (\beta+h)^{-\sigma}\}$. ☐

28.5.5 N-Term Asymptotics and D-Term Estimate

Consider now N-terms assuming that A' is a minimizer.

Case $M=1$

Assume first that $M=1$.

(a) Consider first singular and regular zones (but not the boundary zone). Then after rescaling the contribution of ℓ-element to the remainder does not exceed

$$C\bigl(h_1^{-2} + h_1^{-\frac{5}{3}}\nu_1^{\frac{2}{3}}\bigr) \tag{28.5.48}$$

and summation over zone $\{x\colon \ell(x)\le 1\}$ results in the value of this as $\ell=1$ i.e.

$$C\bigl(h^{-2}+h^{-\frac{5}{3}}\nu^{*\,\frac{2}{3}}\bigr),\qquad \nu^* = (\kappa\beta)^{\frac{10}{9}}h^{\frac{4}{9}}|\log h|^K. \tag{28.5.49}$$

Recall that for $\ell \ge 1$ we have $h_1 = h\ell$, $\beta_1 = \beta\ell^3$ and ν_1 is defined by (28.5.31) which is sufficient even without invoking Remark 28.5.9 since all powers of ℓ in (28.5.48) become negative. Therefore the contribution of the regular exterior zone also does not exceed (28.5.49).

(b) Consider now the boundary zone. Let us repeat arguments used in the proof of Proposition 28.5.12: the contribution of γ-element does not exceed $C\beta_2\bigl(h_2^{-1} + h_2^{-\frac{2}{3}}\nu_2^{\frac{2}{3}}\bigr)$ and plugging $\beta_2 = \beta_1\gamma^{-1}$, $h_2 = h_1\gamma^{-3}$ and $\nu_2 = \nu_1\gamma^{\frac{3}{2}+\delta}$ we get $C\beta_1\bigl(h_1^{-1}\gamma^2 + h_1^{-\frac{2}{3}}\nu_1^{\frac{2}{3}}\gamma^{2+\delta}\bigr)$ and therefore the total contribution of the boundary zone to the remainder does not exceed

$$C\beta_1\int \bigl(h_1^{-1}\gamma^{-1} + h_1^{-\frac{2}{3}}\nu_1^{\frac{2}{3}}\gamma^{-1+\delta}\bigr)\,dx \asymp C\bigl(h_1^{-2}|\log h| + h_1^{-\frac{5}{3}}\nu_1^{\frac{2}{3}}\bigr) \tag{28.5.50}$$

since $\beta_1 = h_1^{-1}$ and from Subsection 26.5.1 we also know that even in the general case

$$\mathsf{D}(\gamma^{-1+s}, \gamma^{-1+s}) \le Cs^{-2} \qquad \text{for}\quad s > 0. \tag{26.5.14}$$

Here we integrate over $\gamma \ge \bar\gamma = h_1^{\frac{1}{3}}$ while the contribution of the zone $\{x\colon \gamma(x) \le \bar\gamma$ does not exceed Ch_1^{-2}.

If $\bar\gamma \ge h_1^{\frac{1}{3}}$ (i.e. $(Z-N)_+ \gtrsim B^{\frac{5}{12}}$) we invoke in the zone $\{x\colon \gamma(x) \le \bar\gamma\}$ the strong non-degeneracy assumption (28.3.60) fulfilled for $M = 1$ and estimate its contribution by the same expression (28.5.50) albeit without the logarithmic term. Similar arguments work also for $(Z-N)_+ \ge B^{\frac{3}{4}}$.

(c) In expression (28.5.50) the logarithmic factor is mildly annoying. However we can get rid of it using our standard propagation arguments like in Subsection 26.6.3; we leave easy details to the reader.

Note that so far in the estimate we also have $P'_{Bh}(V)$ rather than $P'_{\beta h}$; observe however that in the virtue of non-degeneracy assumption (28.3.60) fulfilledfor $M = 1$ the error when we replace $P'_{Bh}(V)$ by $P'_{\beta h}(V)$ does not exceed $C\beta_1 h_1^{-1}$ on the regular elements and Ch_2^{-2} on the boundary elements and summation in both cases results in $O(\beta h^{-1}\bar\ell^2) = O(\beta^{\frac{1}{2}}h^{-\frac{3}{2}})$. Therefore in contrast to the trace estimate there is no deterioration.

Scaling back, we arrive to estimate (28.5.51) below.

(d) In the framework of Theorem 28.5.16 we invoke our standard propagation arguments in the zone $\{x\colon (\beta+h)^{\sigma}\le \ell(x)\le (\beta+h)^{-\sigma}\}$; considering D-terms we invoke these arguments if both elements in the pair belong to this zone. Again, we leave easy details to the reader. Scaling back, we arrive to estimate (28.5.53) below.

(e) We deal with D-term in our usual manner considering double partition and different pairs of partition elements–disjoint when we just apply above arguments since the kernel $|x-y|^{-1}$ is smooth there and non-disjoint when we appeal to the local estimates of D-term. We we leave easy details to the reader.

Proposition 28.5.17. *Let $V=W_B^{\mathsf{TF}}+\lambda$ be a Thomas-Fermi potential for $B\le Z^{\frac{4}{3}}$, $N\asymp Z$ and $M=1$. Then*

(i)

$$|\int \bigl(\operatorname{tr} e(x,x,0)-P'_B(V(x)\bigr)\,dx|\le CR \tag{28.5.51}$$

and

$$\mathsf{D}\bigl(\operatorname{tr} e(x,x,0)-P'_B(V(x),\,\operatorname{tr} e(x,x,0)-P'_B(V(x)\bigr)\le CZ^{\frac{1}{3}}R^2 \tag{28.5.52}$$

with

$$R=R_0:=DefZ^{\frac{2}{3}}+Z^{\frac{5}{9}}\nu^{*\,\frac{2}{3}},\qquad \nu^*=(\alpha B)^{\frac{10}{9}}Z^{-\frac{4}{27}}|\log Z|^K. \tag{28.5.53}$$

(ii) In the framework of Theorem 28.5.16 estimates (28.5.51) *and* (28.5.52) *hold with*

$$R:=CZ^{\frac{2}{3}}\bigl(Z^{-\delta}+B^{\delta}Z^{-\delta}+(\alpha Z)^{\delta}\bigr). \tag{28.5.54}$$

Case $M\ge 2$

Consider now $M\ge 2$. In comparison with the case $M=1$ we should get some extra terms because

(a) First, in the regular zone with $\ell(x)\ge \epsilon d$ the strong non-degeneracy assumption (28.3.60) is replaced by the strong assumption (28.3.65).

(b) In the boundary zone with $\gamma(x)\le\bar\gamma$ (and with $\bar\gamma\ge h_1^{\frac{1}{3}}$) there is no non-degeneracy assumption at all.

Consider a regular zone first. According to (28.3.86) we get an extra term

$$C\beta_1 h_1^{-1}\nu_1^{\frac{1}{2}} \asymp C\beta h^{-1}(\kappa\beta)^{\frac{5}{9}}\ell^{\frac{20}{9}}|\log h|^K \tag{28.5.55}$$

since other extra terms are smaller; summation over the regular zone results in the value with $\ell = \bar{r}$; since $\bar{r} = (\beta h)^{-\frac{1}{4}}$ we get $C\kappa^{\frac{5}{9}}\beta h^{-\frac{14}{9}}|\log h|^K$. Scaling back we arrive to

$$CR'' = C\alpha^{\frac{5}{9}} B Z^{\frac{2}{27}}|\log Z|^K. \tag{28.5.56}$$

Using γ-partition in the boundary zone and plugging $h_2 = h_1\gamma^{-3}$, $\beta_2 = \beta_1\gamma^{-1}$, $\nu_2 = \nu_1\gamma^{\frac{3}{2}+\delta}$ (see Remark 28.5.11) and using (28.5.52) we prove easily that if $\bar{\gamma} = h_1^{\frac{1}{3}}$ (i.e. $(Z-N)_+ \le B^{\frac{5}{12}}$) the contribution of the boundary zone is smaller than CR''.

On the other hand, in the case $B^{\frac{5}{12}} \le (Z-N)_+ \le B^{\frac{3}{4}}$ we need to add $C\beta_2 h_2^{-\frac{3}{2}}\bar{\gamma}^{-2}(1+|\log\bar{\gamma}|)$. Plugging $h_2 = h_1\bar{\gamma}^{-3}$, $\beta_2 = \beta_1\bar{\gamma}^{-1}$, $\bar{\gamma} = (Z-N)_+^{\frac{1}{4}}B^{-\frac{3}{16}}$ and scaling back we arrive to

$$CR''' = C(Z-N)_+^{\frac{3}{8}}B^{\frac{11}{32}}\bigl(1+|\log(Z-N)_+B^{-\frac{3}{4}}|\bigr). \tag{28.5.57}$$

Finally if $(Z-N)_+ \ge B^{\frac{3}{4}}$ we get $C\beta_1 h_1^{-\frac{3}{2}}$ with $\ell = (Z-N)_+^{-\frac{1}{3}}Z^{\frac{1}{3}}$ i.e.

$$CR''' = C(Z-N)_+^{-\frac{1}{2}}B. \tag{28.5.58}$$

Thus we arrive to Proposition 28.5.18(i). The similar arguments work for D-term and we arrive to Proposition 28.5.18(ii)

Proposition 28.5.18. *Let $V = W_B^{\mathsf{TF}} + \lambda$ be a Thomas-Fermi potential with $B \le Z^{\frac{4}{3}}$, $N \asymp Z$ and $M \ge 2$. Let $d \ge Z^{-\frac{1}{3}}$. Then*

(i) Estimate (28.5.51) *holds with $R = R_0 + R''$ and R'' defined by* (28.5.56) *for $(Z-N)_+ \le B^{\frac{5}{12}}$, $R = R_0 + R'' + R'''$ and R''' defined by* (28.5.57) *for $B^{\frac{5}{12}} \le (Z-N)_+ \le B^{\frac{3}{4}}$, $R = R_0 + R'''$ and R''' defined by* (28.5.58) *for $(Z-N)_+ \ge B^{\frac{3}{4}}$.*

Furthermore, if $B \le Z$ estimate (28.5.51) *holds with*

$$R = Z^{\frac{2}{3}}\bigl[Z^{-\delta} + B^{\delta}Z^{-\delta} + (dZ^{\frac{1}{3}})^{-\delta} + (\alpha Z)^{\delta}\bigr]. \tag{28.5.59}$$

(ii) The left-hand expression of (28.5.57) *does not exceed* $CZ^{\frac{1}{3}}R_0^2 + CB^{\frac{1}{4}}R''^2$ *if* $(Z-N)_+ \le B^{\frac{5}{12}}$, $CZ^{\frac{1}{3}}R_0^2 + CB^{\frac{1}{4}}(R''+R''')^2$ *and* R''' *defined by* (28.5.57) *if* $B^{\frac{5}{12}} \le (Z-N)_+ \le B^{\frac{3}{4}}$, $CZ^{\frac{1}{3}}R_0^2 + (Z-N)_+^{\frac{1}{3}}R'''^2$ *and* R''' *defined by* (28.5.58) *if* $(Z-N)_+ \ge B^{\frac{3}{4}}$.

Furthermore, if $B \le Z$ *the left-hand expression of* (28.5.57) *does not exceed* $CZ^{\frac{1}{3}}R^2$ *with* R *defined by* (28.5.59).

28.5.6 More Estimates to a Minimizer

Now we want to provide different kinds of estimates to the minimizer for $\ell(x) \ge Z^{-\frac{1}{3}}$ in the original scale. More precisely, we are looking for

$$\alpha^{-1}\int \phi_r(x)|\partial A'|^2\,dx \tag{28.5.60}$$

with ϕ_r supported in $\{x\colon \ell(x)\asymp r\}$ because it will appear as an error when we decouple singularities for $M\ge 2$ (in this case we should take $r\asymp d$. Due to equation (27.2.14) it is D-type term as well: namely, with the integral taken over $\mathbb{R}^3$ it would be equal to $\alpha Z^{\frac{5}{3}}\mathsf{D}(\phi\Phi_j,\phi\Phi_j)$ calculated in the rescaled coordinates with Φ_j defined by (27.2.14); however with the cut-off the integral kernel $|x-y|^{-1}$ needs to be modified. Recall that the corresponding Weyl expression is 0.

First, using (28.5.16) and decomposition like in the proof of Proposition 27.3.9 we can rewrite (28.5.60) as

$$I := \int K(z;x,y)\Phi(x)\Phi(y)\,dxdydz \tag{28.5.61}$$

multiplied by $\alpha Z^{\frac{5}{3}}$; here $K(z;x,y)$ is supported in $\{z\colon \ell(z)\asymp r\}$, singular at $x=z$ and $y=z$ and satisfies

$$|K(z;x,y)| \le |x-z|^{-2}|y-z|^{-2}|x|\cdot|y|(|x|+r)^{-1}(|y|+r)^{-1}. \tag{28.5.62}$$

Here we temporarily replaced r by $Z^{\frac{1}{3}}r$.

Let us make a double ℓ-admissible partition of unity and consider pairs of elements with $\ell(x)\asymp r_1$ and $\ell(y)\asymp r_2$. There are three cases: $r_1\le \epsilon r$, $r_1\asymp r$ and $r_1\ge cr$, and so also for r_2, and we can consider only pure pairs.

Case $M=1$

Assume first that $M=1$. Then the contribution of each pair with $r_j\le \epsilon r$ (assuming that they belong to regular zone) does not exceed

$$C\zeta_1 r_1\bigl(h_1^{-2}+h_1^{-\frac{5}{3}}\nu_1^{\frac{2}{3}}\bigr)\times \zeta_2 r_2\bigl(h_2^{-2}+h_2^{-\frac{5}{3}}\nu_2^{\frac{2}{3}}\bigr)\times r^{-3}, \tag{28.5.63}$$

where $\zeta_j=r_j^{-2}$, $h_j=hr_j$, $\nu_j=(\kappa\beta)^{\frac{10}{9}}h^{\frac{4}{9}}r_j^{\frac{4}{9}}$ if $r_j\ge 1$ and $\zeta_j=r_j^{-\frac{1}{2}}$, $h_j=hr_j^{-\frac{1}{2}}$, $\nu_j=(\kappa\beta)^{\frac{10}{9}}h^{\frac{4}{9}}$ if $r_j\le 1$. Double summation returns its value if $r_1=r_2=1$ i.e.

$$Ch^{-4}\bigl(1+h^{\frac{2}{3}}\nu^{*\,\frac{4}{3}}\bigr)r^{-3}. \tag{28.5.64}$$

Further, using Fefferman-de Llave decomposition one can prove easily that the contribution of pairs with $r_1\asymp r_2\asymp r$ (the only case when we have a singular kernel) does not exceed (28.5.63) calculated as $r_1=r_2=r$ which is decaying function of r and therefore does not exceed (28.5.64).

Furthermore, the contribution of each pair with $r_j\ge Cr$ (assuming that they belong to regular zone) does not exceed

$$C\zeta_1 r_1^{-2}\bigl(h_1^{-2}+h_1^{-\frac{5}{3}}\nu_1^{\frac{2}{3}}\bigr)\times \zeta_2 r_2^{-2}\bigl(h_2^{-2}+h_2^{-\frac{5}{3}}\nu_2^{\frac{2}{3}}\bigr)\times r^{3}, \tag{28.5.65}$$

and the double summation returns its value with $r_1=r_2=r$ which is the same as (28.5.63) calculated with $r_1=r_2=r$ and again does not exceed (28.5.64).

Finally, considering $r_1\asymp r_2\asymp \bar{r}$ we apply for $(Z-N)_+\le B^{\frac{3}{4}}$ secondary partitions with respect to x and y and using our standard arguments we estimate the contribution of this zone by (28.5.65) calculated with $r_1=r_2=\bar{r}$.

Therefore we estimated expression (28.5.61) by (28.5.64). In particular, if $\kappa\beta\le h^{-\frac{17}{20}}|\log h|^{-K}$ i.e. $\alpha B\le Z^{\frac{17}{60}}|\log Z|^{-K}$), then $\nu^*\le h^{-\frac{1}{2}}$ and expression (28.5.61) does not exceed $Ch^{-4}r^{-3}$. Plugging $h=Z^{-\frac{1}{3}}$, multiplying by $\alpha Z^{\frac{5}{3}}$ and replacing r by $Z^{\frac{1}{3}}r$ we get $\alpha Z^2 r^{-3}$ thus proving Proposition 28.5.19(i).

On the other hand, for $\kappa\beta\ge h^{-\frac{17}{20}}|\log h|^{-K}$ estimate (28.5.61) by (28.5.64) could be improved. Indeed, let us apply all the above arguments only for $r_j\ge t$ with $1\le t\le \epsilon r$. Then we get expression (28.5.63) with $r_1=r_2=t$ i.e.

$$Ch^{-4}\times \nu^{*\,\frac{4}{3}}h^{\frac{2}{3}}t^{-\frac{128}{27}}r^{-3} \tag{28.5.66}$$

where we consider only term possibly exceeding $Ch^{-4}r^{-3}$.

To estimate the contribution of zone $\{x, y\colon \ell(x) \le t, \ell(y) \le t\}$ we replace Φ_j by $(\kappa h^{-2})\Delta A'_j$ and using the standard estimate for operator norm in $\mathscr{L}^2$ we conclude that the corresponding part of expression (28.5.61) does not exceed $C\kappa^{-2}h^{-4}\|\partial A'\|^2 \times t^3 r^{-3} \le Ch^{-4}t^3r^{-3}$ as long as $\|\partial A'\| \le C\kappa$.

Adding this to (28.5.66) and minimizing by $t \lesssim r$ we get $Ch^{-4}(\nu^{*2}h)^{\frac{54}{209}}r^{-3}$ provided $r \ge (\nu^{*2}h)^{\frac{18}{209}}$.

Plugging ν^* and h, multiplying by $\alpha Z^{\frac{5}{3}}$ and replacing r by $Z^{\frac{1}{3}}r$ we arrive to Proposition 28.5.19(ii).

Proposition 28.5.19. *Let $V = W_B^{\mathsf{TF}} + \lambda$ be a Thomas-Fermi potential with $B \le Z^{\frac{4}{3}}$, $N \asymp Z$ and $M = 1$. Then*

(i) A minimizer satisfies

$$\alpha^{-1}\int_{\{x\colon \ell(x)\ge r\}} |\partial A'|^2\, dx \le CT_0 r^{-3} = C\alpha Z^2 r^{-3} \tag{28.5.67}$$

for $r \ge r_* = Z^{-\frac{1}{3}}$ holds provided

$$\alpha B \le Z^{\frac{17}{60}} |\log Z|^{-K}. \tag{28.5.68}$$

(ii) Otherwise a minimizer satisfies

$$\alpha^{-1}\int_{\{x\colon \ell(x)\ge r\}} |\partial A'|^2\, dx \le CT_0 r^{-3} = C\alpha Z^3 r_*^3 r^{-3} \qquad \textit{for} \quad r \ge r_* \tag{28.5.69}$$

with

$$r_* := (\alpha B)^{\frac{40}{209}} Z^{-\frac{81}{209}} |\log Z|^K \gtrsim Z^{-\frac{1}{3}}. \tag{28.5.70}$$

Remark 28.5.20. (i) Assumption (28.5.68) means exactly that $r_* \le Z^{-\frac{1}{3}}$.

(ii) Our usual approach implies that for $B \le Z$ the Tauberian error estimate could be slightly improved but it has no implications here because in contrast to $e(x, x, \tau)$ where the main term in the formal asymptotic decomposition is $h^{-3}P'_{Bh}$ and the next one is $\asymp \beta^2 h^{-2}$, in Φ_j the main term is 0 and the next one is ηh^{-2} with the coefficient η depending on A' and trying to calculate it and plug the corresponding term into (28.5.61) instead of Φ_j will certainly result in the identity.

(iii) It may happen that $r_* \ge \bar{r}$; then it follows from the proof that r_* should be truncated to $\bar{r}$ in (28.5.69). Moreover, estimate (28.5.69) with $r_* = \bar{r}$ holds even for $M \ge 2$ if no non-degeneracy assumption is made.

Case $M\geq 2$

Assume now that $M\geq 2$ and that (28.5.19) is fulfilled. Then we need to take into account excess terms in our estimates. In the regular zone such excess term is

$$C\zeta_1 r_1\beta_1 h_1^{-1}\nu_1^{\frac{1}{2}}\times \zeta_2 r_2\beta_2 h_2^{-1}\nu_2^{\frac{1}{2}}\times r^{-3}\qquad \text{for}\quad r_1\leq r, r_2\leq r \tag{28.5.71}$$

and

$$C\zeta_1 r_1^{-2}\beta_1 h_1^{-1}\nu_1^{\frac{1}{2}}\times \zeta_2 r_2^{-2}\beta_2 h_2^{-1}\nu_2^{\frac{1}{2}}\times r^{3}\qquad \text{for}\quad r_1\geq r, r_2\geq r. \tag{28.5.72}$$

Plugging β_j, h_j and ν_j one observes easily that the former is a growing and the latter is a decaying function of r_j and these expressions coincide at $r_1=r_2=r$. To decouple singularities we need to consider $r\leq \epsilon d$ where d is the minimal distance between singularities; so we will assume this. Observe that extra terms appear only if $r_j\geq \epsilon d$, so we need to consider only (28.5.72).

Therefore if $d\leq \bar{r}$ the summation results in expression (28.5.72) calculated at $r_1=r_2=d$ which is

$$C\beta^2 h^{-\frac{14}{9}}(\kappa\beta)^{\frac{10}{9}}|\log h|^K d^{-\frac{32}{9}} r^3,$$

which results in the original settings in[33)]

$$CT' r^3 = C(\alpha B)^{\frac{19}{9}} B d^{-\frac{32}{9}} r^3; \tag{28.5.73}$$

recall that we plug β, h, κ, replace d and r by $Z^{\frac{1}{3}}d$ and $Z^{\frac{1}{3}}r$, and multiply by $\alpha Z^{\frac{5}{3}}$.

Meanwhile, using our standard arguments one can prove easily that the contribution of the boundary zone is less than this provided $(Z-N)_+\leq B^{\frac{5}{12}}$.

On the other hand, for $B^{\frac{5}{12}}\leq (Z-N)_+\leq B^{\frac{3}{4}}$ an extra contribution of the boundary zone does not exceed

$$C\beta^2 h^{-3}\bar{\gamma}^{13}\bar{r}^{-5} r^3 (1+|\log\bar{\gamma}|)^2,$$

which results in the original settings in[33)]

$$CT'' r^3 = C\alpha (Z-N)_+^{\frac{13}{4}} B^{\frac{13}{16}}\bigl(1+|\log (Z-N)_+ B^{-\frac{3}{4}}|\bigr)^2 r^3. \tag{28.5.74}$$

[33)] I.e. after we plug κ,β,h, replace d and r by $Z^{\frac{1}{3}}d$ and $Z^{\frac{1}{3}}r$ and multiply by $\alpha Z^{\frac{5}{3}}$.

Finally, for $(Z-N)_+ \ge B^{\frac{3}{4}}$ an extra contribution of the boundary zone does not exceed

$$C\beta^2 h^{-3}\bar{r}^{-5} r^3,$$

which results in the original settings in[33)]

$$CT'' r^3 = C\alpha (Z-N)_+^{\frac{5}{3}} B^2. \tag{28.5.75}$$

Thus we have proven

Proposition 28.5.21. *Let $V = W_B^{\mathsf{TF}} + \lambda$ be Thomas-Fermi potential with $B \le Z^{\frac{4}{3}}$, $N \asymp Z_1 \asymp Z_2 \asymp \dots \asymp Z_M$ and $M \ge 2$. Let $r_* \ll r \ll d \le \epsilon \bar{r}$.*

Then expression

$$\alpha^{-1} \int_{\{x:\, \ell(x) \asymp r\}} |\partial A'|^2\, dx \tag{28.5.76}$$

does not exceed $C\bigl(T_0 r^{-3} + (T' + T'')r^3\bigr)$ with T_0 defined by (28.5.68) *or* (28.5.69) *and T' defined by* (28.5.73)*, and T'' either 0 (as $(Z-N)_+ \le B^{\frac{5}{12}}$) or defined by* (28.5.74)*, or* (28.5.75)*.*

Remark 28.5.22. (i) Recall that the decoupling error between the singularity and the regular part does not exceed $C\alpha B Z^{\frac{5}{3}}$.

(ii) Meanwhile in these settings $\mathsf{Scott} - \mathsf{Scott}_0 = O(\alpha Z^3)$ and if decoupling error is greater than this there is no point in decoupling.

(iii) Obviously we need to assume that $r_* \le \epsilon \bar{r}$ which implies that

$$(\alpha Z)^{40} B^{\frac{369}{4}} \le \epsilon Z^{121}, \tag{28.5.77}$$

which is just tiny bit stronger than $\alpha Z \lesssim 1$, $B \lesssim Z^{\frac{4}{3}}$. For $(Z-N)_+ \le B^{\frac{3}{4}}$ this condition is also sufficient.

(iv) Decoupling singularities we get an error (28.5.76) with integration over $\{x\colon \ell(x) \asymp r\}$; therefore if $r_* \ll d \le \bar{r}$ then minimizing $T_0 r^{-3} + T' r^3$ by $r : r_* \le r \le d$ we get

$$T_* := \bigl(T_0 (T' + T'')\bigr)^{\frac{1}{2}} + (T' + T'') r_*^3 + T_0 d^{-3}. \tag{28.5.78}$$

28.5.7 Endgame: $M \ge 2$

For $M \ge 2$ we have two rather different results. In the first (28.5.39) we appeal to the sum of localized trace terms $\sum_{1\le m\le M} \mathsf{Tr}(\psi_m H^-_{A,V_m}\psi_m)$ where ψ_m is supported in $\{x\colon |x - \mathsf{y}_m| \le \frac{1}{3}d\}$ (recall that d is the minimal distance between singularities).

In the second one we want to use $2h^{-2}\sum S(\alpha Z_m)Z_m^2$ instead. If $A' = 0$ then transition would be immediate. However in our case we need to "decouple" singularities. Therefore in the estimate from below we need results from the previous subsubsection:

Theorem 28.5.23. *Let $V = W_B^{\mathsf{TF}} + \lambda$ be a Thomas-Fermi potential with $B \le Z^{\frac{4}{3}}$, $N \asymp Z$ and $M \ge 2$. Let $\kappa = \alpha Z \le \kappa^*$. Then if $r_* \le d \le \bar{r}$*

$$|\mathsf{E}^*_\alpha + \int P_B(V)\, dx - 2\sum S(\alpha Z_m)Z_m^2 - \mathsf{Schwinger}| \tag{28.5.79}$$

does not exceed $C(Q + T)$ where Q is the trace estimate obtained in Proposition 28.5.12(iii)–(iv) and T_* is an estimate for expression (28.5.76) *given by* (28.5.78).

Proof. (i) In the estimate from below we just replace A' in $\mathsf{E}_\alpha(A)$ by the sum $\sum_{1\le m\le M} A'\psi_m$ with ψ_m supported in $\{x\colon |x - \mathsf{y}_m| \le \frac{1}{3}r\}$ and equal 1 in $\{x\colon |x - \mathsf{y}_m| \le \frac{1}{4}r\}$ where r is the minimal distance between singularities, and observe that $\alpha^{-1}\|\partial A'\|^2$ increased by no more than CT.

(ii) In the estimate from above we just plug into $\mathsf{E}_\alpha(A)$ $A' = \sum_{1\le m\le M} A'_m\psi_m$ with A'_m minimizers for a single-singularity potential V_m. □

Remark 28.5.24. (i) Theorem 28.5.23 makes sense only if $r_* \ll d \le \bar{r}$ and $T_* \ll \alpha Z^3$; if any of these assumptions fails, we observe that $\mathsf{E}_\alpha(A')$ is greater than $\mathcal{E}_0 + \mathsf{Schwinger} - CQ - C\alpha Z^3$ and in this case we can replace $S(\alpha Z_m)$ by $S(0)$; in this case in the upper estimate we pick up $A' = 0$.

(ii) In the estimate from above $T = \max_m T_m$ with T_m an estimate for a single-singularity potential V_m delivered by Proposition 28.5.19; thus $T = T_0 d^{-3}$ if $r_* \le d \le \bar{r}$. Still it is at least $C\alpha B^{\frac{3}{4}}Z^2$ while decoupling error of singularity and the regular zone is $C\alpha BZ^{\frac{5}{3}}$ which is smaller.

28.6 Global Trace Asymptotics in the Case of Thomas-Fermi Potential: $Z^{\frac{4}{3}} \le B \le Z^3$

28.6.1 Trace Estimates

In this Section we consider the case of $Z^{\frac{4}{3}} \le B \le Z^3$ (corresponding to $\beta h \ge 1$ after rescaling[34)]). We start with

Remark 28.6.1. (i) In contrast to the previous Section 28.5 in this case the remainder estimate will be at least $C\kappa h^{-2}$ and therefore there will be no difficulty to decouple between singularities or between singularities and a regular zone and the Scott correction term will be either $\sum 2S(0)Z_m^2$ or even absent.

Therefore in the estimate from above we just pick up $A'=0$ both here and in the multiparticle problem and we will need only N-term and D-terms with $A'=0$ referring to Chapter 25.

(ii) For $\beta h \ge 1$ we have a major dichotomy unrelated to the self-generated magnetic field:

(a) $\beta h^2 \le 1$ (i.e. $Z^{\frac{4}{3}} \le B \le Z^{\frac{7}{4}}$). In this case Scott correction term could be larger than the contribution of zone $\{x\colon \ell(x) \asymp 1\}$ to the remainder estimate which is no better than $O(\beta)$ and one probably needs to include Scott correction term in the final trace asymptotics.

(b) $\beta h^2 \ge 1$ (i.e. $Z^{\frac{7}{4}} \le B \le Z^3$). In this case the opposite is true; then one does not need to include Scott correction term for sure. Recall that condition $C \le Z^3$ is also unrelated to self-generated magnetic field.

(iii) Recall that we need to impose condition $\kappa\beta h^2|\log\beta|^K \le 1$ which is equivalent to

$$\alpha B^{\frac{4}{5}} Z^{-\frac{2}{5}} |\log Z|^K \le 1. \tag{28.6.1}$$

---

34) Recall that as $Z^{\frac{4}{3}} \lesssim B \lesssim Z^3$ the scaling is $x \mapsto B^{\frac{2}{5}} Z^{-\frac{1}{5}} x$ (and the original distance between nuclei is at least $B^{-\frac{2}{5}} Z^{\frac{1}{5}}$), $\tau \mapsto B^{-\frac{2}{5}} Z^{\frac{4}{5}} \tau$, $\beta = B^{\frac{2}{5}} Z^{-\frac{1}{5}}$, $h = B^{\frac{1}{5}} Z^{-\frac{3}{5}}$ and $B \lesssim Z^3$.

35) Cf. Proposition 28.5.2.

Theorem 28.6.2 [35)]**.** *Let V be Thomas-Fermi potential $V := W_B^{\mathsf{TF}} + \lambda$ with $Z^{\frac{4}{3}} \le B \le Z^3$, $N \asymp Z_1 \asymp Z_2 \asymp \dots \asymp Z_M$ and $N \le Z$. Let $\alpha Z \le \kappa^*$ and assumption* (28.6.1) *be fulfilled. Let A' be a minimizer. Then*

(i) If <u>either</u> $(Z-N)_+ \lesssim B^{\frac{4}{15}} Z^{\frac{1}{5}}$ <u>or</u> $M=1$ and $\alpha B^{\frac{3}{5}} Z^{\frac{1}{5}} \gtrsim 1$, then expression

$$|\mathsf{E}_\kappa(A') - \mathsf{Scott}_0 + \int\int P_B(V(x))\,dx| \tag{28.6.2}$$

does not exceed

$$C\Bigl(B^{\frac{1}{3}} Z^{\frac{4}{3}} + B^{\frac{4}{5}} Z^{\frac{3}{5}} + \alpha Z^3 + \alpha^{\frac{16}{9}} B^{\frac{82}{45}} Z^{\frac{58}{45}} |\log Z|^K\Bigr). \tag{28.6.3}$$

(ii) If $M=1$, $(Z-N)_+ \gtrsim B^{\frac{4}{15}} Z^{\frac{1}{5}}$ and $\alpha B^{\frac{3}{5}} Z^{\frac{1}{5}} \lesssim 1$, then expression (28.6.2) *does not exceed*

$$\begin{aligned} C\Bigl(&B^{\frac{1}{3}} Z^{\frac{4}{3}} + B^{\frac{4}{5}} Z^{\frac{3}{5}} + \alpha Z^3 + \alpha^{\frac{16}{9}} B^{\frac{82}{45}} Z^{\frac{49}{45}} |\log Z|^K \\ &+ \alpha^{\frac{40}{27}} B^{\frac{74}{45}} Z^{\frac{131}{540}} (Z-N)_+^{\frac{85}{108}} |\log Z|^K\Bigr). \end{aligned} \tag{28.6.4}$$

(iii) If $M \ge 2$ and $(Z-N)_+ \gtrsim B^{\frac{4}{15}} Z^{\frac{1}{5}}$, then expression (28.6.2) *does not exceed*

$$\begin{aligned} C\Bigl(&B^{\frac{1}{3}} Z^{\frac{4}{3}} + B^{\frac{4}{5}} Z^{\frac{3}{5}} + \alpha Z^3 + \alpha^{\frac{16}{9}} B^{\frac{82}{45}} Z^{\frac{49}{45}} |\log Z|^K \\ &+ B^{\frac{7}{10}} Z^{\frac{11}{40}} (Z-N)_+^{\frac{5}{8}} |\log (Z-N)_+ Z^{-1}|\Bigr). \end{aligned} \tag{28.6.5}$$

Proof. (a) Observe first that we need to prove only the estimate from below for expression (28.6.2) without absolute value since in the estimate from above we just pick $A'=0$ and apply results of Chapter 25 producing estimate $CB^{\frac{4}{5}} Z^{\frac{3}{5}}$.

Proof of the estimate from below repeats the proof of Proposition 28.5.2. Namely, we apply an appropriate partition and on each element ψ_ι^2 estimate from below

$$\mathsf{Tr}^-(\psi_\iota H_{A,V} \psi_\iota) + (C_0\alpha)^{-1} \int |\partial A'|^2\,dx + \int\int P_B(V(x))\psi_\iota^2(x)\,dx \tag{28.6.6}$$

for $\iota \ge 1$ and

$$\mathsf{Tr}^-(\psi_0 H_{A,V}\psi_0) + (C_0\alpha)^{-1}\int |\partial A'|^2\,dx + \iint P_B(V(x))\psi_0^2(x)\,dx - \mathsf{Scott}_0. \tag{28.6.7}$$

For $B \le Z^2$ we separate zone $\mathcal{X}_0 := \{x\colon \ell(x) \le r_* = B^{-\frac{2}{3}}Z^{\frac{1}{3}}\}$ in which after rescaling $x \mapsto r_*^{-1}x$, $\tau \mapsto r_* Z^{-1}\tau$, we have $\beta = 1$, $h = B^{\frac{1}{3}}Z^{-\frac{2}{3}}$ and $\kappa = \alpha Z$. Then for the corresponding partition element ψ_0^2 expression (28.6.7) in virtue of Chapter 26 does not exceed (by an absolute value)

$$C\bigl(h^{-1} + \kappa|\log\kappa|^{\frac{1}{3}}h^{-\frac{4}{3}}\bigr) \times Zr_*^{-1},$$

which does not exceed (28.6.3) without the last term.

For $B \ge Z^2$ we separate zone $\mathcal{X}_0 := \{x\colon \ell(x) \le r_* = Z^{-1}\}$ and after rescaling $x \mapsto r_*^{-1}x$, $\tau \mapsto Z^{-1}r_*\tau$ we have $h = 1$, $\beta = BZ^{-2}$ and apply variational estimates of Appendix 28.A.1 here. Then the contribution of $\mathcal{X}_0$ to the remainder does not exceed $C\beta \times Zr_*^{-1} = CB \le CB^{\frac{4}{5}}Z^{\frac{3}{5}}$.

(b) Further, a contribution of each regular element with $r_* \le \ell(x) \le \epsilon\bar{r}$ (recall that $\bar{r} = B^{-\frac{2}{5}}Z^{\frac{1}{5}}$) does not exceed

$$C\zeta^2 h_1^{-1}\Bigl(1 + (\kappa_1\beta_1)^{\frac{40}{27}}h_1^{\frac{34}{27}}|\log h_1|^K\Bigr) \qquad \text{for}\quad \beta_1 h_1 \le C_0, \tag{28.6.8}$$

$$C\zeta^2\beta_1\,\Bigl(1 + (\kappa_1\beta_1)^{\frac{16}{9}}h_1^{\frac{14}{9}}|\log h_1|^K\Bigr) \qquad \text{for}\quad \beta_1 h_1 \ge C_0 \tag{28.6.9}$$

with $\zeta = Z^{\frac{1}{2}}\ell^{-\frac{1}{2}}$, $\beta_1 = BZ^{-\frac{1}{2}}\ell^{\frac{3}{2}}$, $h_1 = Z^{-\frac{1}{2}}\ell^{-\frac{1}{2}}$, $\kappa_1 = \alpha Z$. Indeed, if $\beta_1 h_1 \ge C_0$ and $\ell(x) \le \epsilon\bar{r}$, then the super-strong non-degeneracy assumption (28.4.5) is fulfilled.

Observe that the first term in (28.6.8) has ℓ in the negative power and therefore sums to its value at $\ell = r_*$ while the second term has ℓ in the positive power and therefore sums to its value at $\beta_1 h_1 = 1$ (i.e. $\ell = B^{-1}Z$, $h_1 = B^{\frac{1}{2}}Z^{-1}$, $\beta_1 = B^{-\frac{1}{2}}Z$); one can see easily that it is less than αZ^3. Actually this zone appears only as $B \le Z^2$.

On the other hand, both terms in (28.6.9) have ℓ in the positive power and thus sum to their values at $\ell = \bar{r}$, $\beta_1 = B^{\frac{2}{5}}Z^{-\frac{1}{5}}$, $h_1 = B^{\frac{1}{5}}Z^{-\frac{3}{5}}$ and $\kappa_1 = \alpha Z$ which are exactly the second and the fourth terms in (28.6.2).

(c) *Boundary zone* $\{x\colon \epsilon \le \ell(x) \le c\}$ is treated in the same way albeit with $\zeta = B^{\frac{2}{5}} Z^{\frac{4}{5}}\gamma^2$, $\beta_1 = B^{\frac{2}{5}} Z^{-\frac{1}{5}}\gamma^{-1}$, $h_1 = B^{\frac{1}{5}} Z^{-\frac{3}{5}}\gamma^{-3}$ and $\kappa_1 = \alpha Z\gamma^5$ as long as $\gamma \ge C_0\bar{\gamma}$ (with $\bar{\gamma} = (Z-N)_+^{\frac{1}{4}} Z^{-\frac{1}{4}}$ but reset to $B^{\frac{1}{15}} Z^{-\frac{1}{5}}$ if the latter is larger). Observe that plugging into (28.6.9) we get in both terms γ in the power greater than 2; therefore after summation with respect to partition elements we get expression (28.6.9) with $\gamma = 1$, $\beta_1 = B^{\frac{2}{5}} Z^{-\frac{1}{5}}$, $h_1 = B^{\frac{1}{5}} Z^{-\frac{3}{5}}$ and $\kappa_1 = \alpha Z$.

This proves the lower estimate (28.6.2) in the framework of the first clause of Statement (i) as contribution of the zone $\gamma \le B^{\frac{1}{15}} Z^{-\frac{1}{5}}$ is estimated easily; we leave it to the reader.

(d) Assume now that $(Z-N)_+ \ge B^{\frac{4}{15}} Z^{\frac{1}{5}}$. We do not partition zone $\{x\colon \gamma(x) \le C_0\bar{\gamma}\}$ further. In this case we need to take

$$\nu_1 = \bigl((\kappa_1\beta_1)^{\frac{4}{3}} h_1^{\frac{2}{3}} + (\kappa_1\beta_1)^{\frac{10}{9}} h_1^{\frac{4}{9}}\bigr)|\log h_1|^K. \tag{28.6.10}$$

For $M=1$ we should plug it into

$$C\zeta^2\beta_1\bigl(1 + h_1^{\frac{2}{3}}\nu_1^{\frac{4}{3}}\bigr)\gamma^{-2} \tag{28.6.11}$$

with $\zeta = B^{\frac{2}{5}} Z^{\frac{4}{5}}\gamma^2$ and $\gamma = \bar{\gamma}$.

For $\kappa\beta h \gtrsim 1$ we estimate it by the same expression with $\bar{\gamma}$ replaced by 1 but then in ν_1 dominates the first term and we arrive to the lower estimate (28.6.2) in the framework of the second clause of Statement (i).

(e) For $M=1$ and $\kappa\beta h \lesssim 1$ we need to take into account term (28.6.11) with $\nu_1 = (\kappa_1\beta_1)^{\frac{10}{9}} h_1^{\frac{4}{9}} |\log h_1|^K$ which results in the last term in (28.6.4). Indeed, as $\gamma(x) \le C_0\bar{\gamma}$ super-strong non-degeneracy condition is not fulfilled.

(f) For $M \ge 2$, we need to take into account term $C\zeta^2\beta_1 h_1^{-\frac{1}{2}}\gamma^{-2}(1 + |\log\gamma|)$ with $\gamma = \bar{\gamma}$ which results in the last term in (28.6.5). This concludes estimate from below. □

Corollary 28.6.3. *In the framework of Theorem 28.6.2(i), (ii), (iii) expression* $\|\partial A'\|^2$ *does not exceed expressions* (28.6.3), (28.6.4) *and* (28.6.5) *respectively, multiplied by* α.

Proof. Indeed, the same estimates hold with α replaced by 2α. □

The same methods lead us to a similar result for $B \lesssim Z^{\frac{4}{3}}$ (we leave the oproof to the reader):

Theorem 28.6.4. *Let V be Thomas-Fermi potential $W_B^{\mathsf{TF}} + \lambda$ with $B \le Z^{\frac{4}{3}}$, $N \asymp Z_1 \asymp Z_2 \asymp \ldots \asymp Z_M$ and $N \le Z$. Let $\alpha Z \le \kappa^*$. Let A' be a minimizer. Then*

(i) If either $(Z-N)_+ \lesssim B^{\frac{5}{12}}$ or $M=1$, then expression

$$|\mathsf{E}_\kappa(A') - \mathsf{Scott}_0 + \int\int P_B(V(x))\,dx| \tag{28.6.12}$$

does not exceed

$$C\Bigl(B^{\frac{1}{3}}Z^{\frac{4}{3}} + Z^{\frac{5}{3}} + \alpha Z^3\Bigr);. \tag{28.6.13}$$

(ii) If $M \ge 2$ and $B^{\frac{5}{12}} \lesssim (Z-N)_+ \lesssim B^{\frac{3}{4}}$, then expression (28.6.12) *does not exceed*

$$C\Bigl(B^{\frac{1}{3}}Z^{\frac{4}{3}} + Z^{\frac{5}{3}} + \alpha Z^3 + B^{\frac{29}{32}}(Z-N)_+^{\frac{5}{8}}|\log(Z-N)_+B^{-\frac{3}{4}}|\Bigr). \tag{28.6.14}$$

(iii) If $M \ge 2$ and $(Z-N)_+ \gtrsim B^{\frac{3}{4}}$, then expression (28.6.12) *does not exceed*

$$C\Bigl(B^{\frac{1}{3}}Z^{\frac{4}{3}} + Z^{\frac{5}{3}} + \alpha Z^3 + B(Z-N)_+^{\frac{1}{2}}\Bigr). \tag{28.6.15}$$

28.6.2 Estimates to a Minimizer

Observe that only terms $B^{\frac{1}{3}}Z^{\frac{4}{3}}$ and αZ^3 are associated with the singularities and they are definitely smaller than $B^{\frac{4}{5}}Z^{\frac{3}{5}}$ if $B \gtrsim Z^{\frac{7}{4}}$. Therefore for $B \gtrsim Z^{\frac{7}{4}}$ we do not expect estimate for $\mathsf{D}(\rho_\Psi - \rho_B,\, \rho_\Psi - \rho_B)$ better than expressions (28.6.3)–(28.6.5).

However for $B \lesssim Z^{\frac{7}{4}}$ to improve such estimate we need to study a minimizer. We assume that the remainder in Theorem 28.6.4 does not exceed $C\bigl(B^{\frac{1}{3}}Z^{\frac{4}{3}} + \alpha Z^3\bigr)$ and therefore

$$\|\partial A'\| \le C\alpha^{\frac{1}{2}}B^{\frac{1}{6}}Z^{\frac{2}{3}} + C\alpha Z^{\frac{3}{2}} \tag{28.6.16}$$

or, after our usual scaling,

$$\|\partial A'\| \le \varsigma := C\bigl(\kappa + \kappa^{\frac{1}{2}}\beta^{\frac{1}{6}}h^{\frac{1}{2}}\bigr). \tag{28.6.17}$$

Observe that for $Z^{\frac{4}{3}} \le B \le Z^2$ we have all zones.

Proposition 28.6.5. *Let V be Thomas-Fermi potential $W_B^{\mathsf{TF}} + \lambda$ rescaled with $Z^{\frac{4}{3}} \le B \le Z^3$, $N \asymp Z_1 \asymp Z_2 \asymp \dots \asymp Z_M$ and $N \le Z$. Further, let $\alpha Z \lesssim 1$ and $\alpha B^{\frac{2}{5}} Z^{-\frac{2}{5}} |\log \beta|^K \lesssim 1$. Then under assumption (28.6.17) the minimizer A' satisfies*

(i) If $\ell \le r_* = h^2$ (i.e. $h_1 \ge 1$) then

$$|\partial^2 A'| \le C\varsigma h^{-5}. \tag{28.6.18}$$

(ii) If $r_* \le \ell \le c(\beta h)^{-1}$ (i.e. $h_1 \le 1$, $\beta_1 h_1 \le c$), then

$$\begin{aligned}|\partial^2 A'| \le C\kappa\Bigl(\varsigma \ell^{-\frac{5}{2}} + \min\bigl(\beta^{\frac{3}{2}} h^{\frac{1}{2}} \ell^{-1},\, \beta^{\frac{1}{2}} \ell^{-\frac{3}{4}}\bigr)\Bigr) |\log \ell / r_*| \\ + C(\kappa\beta)^{\frac{10}{9}} h^{\frac{4}{9}} \ell^{-\frac{19}{9}} |\log \ell / r_*|^K.\end{aligned} \tag{28.6.19}$$

(iii) If $c(\beta h)^{-1} \le \ell \le c$, then

$$\begin{aligned}|\partial^2 A'| \le C\varsigma \ell^{-\frac{5}{2}} + C\kappa \beta^{\frac{1}{2}} \ell^{-\frac{7}{4}} |\log \ell / r_*| \\ + C\Bigl((\kappa\beta)^{\frac{10}{9}} h^{\frac{4}{9}} \ell^{-\frac{19}{9}} + (\kappa\beta)^{\frac{4}{3}} h^{\frac{2}{3}} \ell^{-\frac{5}{6}}\Bigr) |\log \ell / r_*|^K.\end{aligned} \tag{28.6.20}$$

Proof. The proof of these two propositions repeats our standard arguments and is left to the reader. □

These propositions may not provide the best D-term estimate as $\kappa\beta h \le 1$ (i.e. $\alpha B^{\frac{3}{5}} Z^{\frac{1}{5}} \le 1$) and could be improved in virtue of the super-strong non-degeneracy assumption fulfilled at regular elements with $\ell \ge c(\beta h)^{-1}$ and at border elements with $\gamma \ge C_0 \bar{\gamma}$. We want to improve term containing $(\kappa\beta)^{\frac{10}{9}} h^{\frac{4}{8}} \ell^{-\frac{19}{9}}$ in (28.6.20). Assume now that $\beta h^2 \le 1$ and $\kappa\beta h \le 1$ (case we need to cover). Let us consider zone $\{x : (\epsilon_0 \beta h \ge V(x) \ge C_0 |\eta|\}$ where in the corresponding scale super-strong non-degeneracy condition is fulfilled and $\eta = \lambda B^{-\frac{2}{5}} Z^{\frac{1}{5}}$.

Proposition 28.6.6. *Let conditions of Proposition 28.6.5 be fulfilled. Then*

(i) Estimate

$$|\partial^2 A'(x)| \le C\Bigl(\varsigma \ell^{-\frac{5}{2}} + \kappa\beta^{\frac{1}{2}} \ell(x)^{-\frac{7}{4}} + (\kappa\beta)^{\frac{4}{3}} h^{\frac{2}{3}} \ell(x)^{-\frac{5}{6}}\Bigr) |\log h|^K \tag{28.6.21}$$

holds provided

$$\beta h |\log h|^{-\delta} \ge V(x) \ge |\eta| \cdot |\log h|^{\delta} \tag{28.6.22}$$

with arbitrarily small exponent $\delta > 0$.

(ii) Furthermore, if $|\eta|\le |\log h|^{-\delta}$*, then estimate*

$$|\partial^2 A'(x)|\le C\Bigl(\varsigma+\kappa\beta^{\frac{1}{2}}+(\kappa\beta)^{\frac{4}{3}}h^{\frac{2}{3}}+(\kappa\beta)^{\frac{10}{9}}h^{\frac{4}{9}}\bar{\gamma}^{\frac{28}{9}}\Bigr)|\log h|^K \tag{28.6.23}$$

holds provided $|V(x)|\lesssim 1$, $\bar{\gamma}=|\eta|^{\frac{1}{4}}$.

Proof. (i) Let

$$\nu_n(t)=\sup_{\mathcal{X}_n(t)}|\partial^2A'(x)|\ell(x)^{\frac{5}{2}},\qquad \mathcal{X}_n(t)=\{e^{-\epsilon n-1}t\le V(x)\le e^{\epsilon n+1}t\}.$$

Here $\epsilon>0$ is arbitrarily small (but constants may depend on it). Assume that

$$e^{\epsilon n}t\le\epsilon_0,\qquad e^{-\epsilon n}t\ge C_0|\eta|,\qquad e^{\epsilon n}\le|\log h|. \tag{28.6.24}$$

Here first two conditions assure that in $\mathcal{X}_n(t)$ the super-strong non-degeneracy assumption is fulfilled after rescaling and the last condition assures that $\ell(x)$ remains the same (modulo logarithmic factor) here. Then

$$\nu_n(t)\le C\Bigl(\varsigma+\kappa\beta_1^{\frac{1}{2}}+C\kappa_1\beta_1h_1^{\frac{1}{4}}(\nu_{n+1}(t))^{\frac{1}{4}}\Bigr)|\log h|^{K_1} \tag{28.6.25}$$

with $\kappa_1=\kappa$, $\beta_1=\beta r^{\frac{3}{2}}$, $h_1=hr^{-\frac{1}{2}}$, $r=\min(t^{-1},1)$. Indeed, $|\Delta A'|$ in $\mathcal{X}_{n+1/2}(t)$ does not exceed the right-hand expression (without term ς and without logarithmic factor) multiplied by $r^{-\frac{5}{2}}$ and $C\varsigma$ estimates $\mathscr{L}^2$-norm of $\partial A'$ (and we scale it properly). Recall that we scale $x\mapsto x/r$ if $r\le\epsilon_0$ and $x\mapsto x/\gamma$ if $r\asymp 1$ and in the latter case $\beta_1=\beta\gamma^{-1}$, $h_1=h\gamma^{-3}$ and $\kappa_1=\kappa\gamma^5$; the uncertainty due to r or γ defined modulo logarithmic factor compensates by $|\log h|^{K_1}$ in the right-hand expression of (28.6.25).

Therefore

$$F_n(t)\le C\Bigl(\varsigma r^{-\frac{5}{3}}+C\kappa\beta^{\frac{1}{2}}r^{-\frac{11}{12}}+C\kappa\beta h^{\frac{1}{2}}\times(F_{n+1}(t))^{\frac{1}{4}}\Bigr)|\log h|^{K_1}$$

for $F_n(t)=\nu_n(t)r^{-\frac{5}{3}}$. Iterating we see that

$$F_0(t)\le C\Bigl(\varsigma r^{-\frac{5}{3}}+\kappa\beta^{\frac{1}{2}}r^{-\frac{11}{12}}\Bigr)|\log h|^K+C(\kappa\beta h^{\frac{1}{2}})^{\frac{4}{3}}|\log h|^K\times\underbrace{(F_{n+1}(t))^{\frac{1}{4^n}}}.$$

Since $F_{n+1}(r)\le h^{-L}$ the last factor is bounded by a constant if $2^n\ge|\log h|$ and we can satisfy this and (28.6.24) as long as (28.6.22) holds. This proves Statement (i).

(ii) Consider the remaining zone $\mathcal{Y} = \{x\colon V(x) \le |\eta|\cdot|\log h|^{\delta}\}$ and let $\nu = \sup_{\mathcal{Y}} |\partial^2 A'|$. Observe that in $\mathcal{Y}$ $|\Delta A'|$ does not exceed

$$C\Bigl(\kappa\beta^{\frac{1}{2}} + \kappa\beta h^{\frac{1}{2}}|\nu|^{\frac{1}{4}} + \kappa\beta h^{\frac{2}{5}}\bar{\gamma}^{\frac{14}{5}}\nu^{\frac{1}{10}}\Bigr)|\log h|^{K}$$

and on its border (28.6.23) is fulfilled. It implies that (28.6.23) is fulfilled in $\mathcal{Y}$ as well. This proves Statement (ii). □

Remark 28.6.7. If $|\eta| \ge |\log h|^{-\delta}$ then Proposition 28.6.5 is sufficiently good in the remaining zone $\mathcal{Y}$.

28.6.3 N-Term Asymptotics and D-Term Estimates

We leave to the reader not complicated but rather tedious and error-prone task

Problem 28.6.8. Estimate remainder in N-term

$$|\int \bigl(e(x,x,\lambda') - P_B(V(x)+\lambda')\bigr)\,dx| \tag{28.6.26}$$

and D-term

$$\mathsf{D}\bigl(e(x,x,\lambda') - P_B(V(x)+\lambda'),\, e(x,x,\lambda') - P_B(V(x)+\lambda')\bigr). \tag{28.6.27}$$

After usual rescaling one needs to consider the following zones:

(a) Zone $\{x\colon \ell(x) \le (\beta h)^{-1}|\log h|^{\delta}\}$. In this zone one should use $\beta_1 = \beta\ell^{\frac{3}{2}}$, $h_1 = h\ell^{-\frac{1}{2}}$ and $\nu_1 = (\kappa\beta_1)^{\frac{10}{9}} h_1^{\frac{4}{9}}|\log h_1|^{K}$ (other terms are not important here); then its contributions to expressions (28.6.26) and (28.6.27) do not exceed respectively $C\bigl(h_1^{-2} + h_1^{-\frac{5}{3}}\nu_1^{\frac{2}{3}}\bigr)$ and $C\bigl(h_1^{-2} + h_1^{-\frac{5}{3}}\nu_1^{\frac{2}{3}}\bigr)^2\ell^{-1}$ (for $\ell(x) \lesssim (\beta h)^{-1}$ but slight extension just adds some logarithmic factor). In the final tally $\ell = (\beta h)^{-1}|\log h|^{\delta}$.

(b) Zone $\{x\colon (\beta h)^{-1}|\log h|^{\delta} \le \ell(x) \le |\log h|^{-\delta}\}$. In this zone we have the same expressions for h_1 and β_1 and $\nu_1 = (\kappa\beta_1)^{\frac{4}{3}} h_1^{\frac{2}{3}}|\log h_1|^{K}$; then its contributions to expressions (28.6.26) and (28.6.27) do not exceed respectively $C\beta_1\bigl(h_1^{-1} + h_1^{-\frac{2}{3}}\nu_1^{\frac{2}{3}}\bigr)$ and $C\beta_1^2\bigl(h_1^{-1} + h_1^{-\frac{2}{3}}\nu_1^{\frac{2}{3}}\bigr)^2\ell^{-1}$. In the final tally $\ell = 1$.

(c) Zone $\{x\colon \ell(x)\ge |\log h|^{-\delta},\ \gamma(x)\ge \bar\gamma|\log h^{\delta}\}$. In this zone $h_1=h\gamma^{-3}$ and $\beta_1=\beta\gamma^{-1}$ and $\nu=(\kappa\beta)^{43}h^{\frac{2}{3}}|\log h|^K$ but we use according to Remark 28.5.9 instead $\nu_1=\kappa_1\beta_1 h_1^{\frac{1}{4}}\nu^{\frac{1}{4}}$ with $\kappa_1=\kappa\gamma^5$. Then

(c_1) For $M=1$ contributions of γ-element to expressions (28.6.26) and (28.6.27) do not exceed $C\beta_1\bigl(h_1^{-1}+h_1^{-\frac{2}{3}}\nu_1^{\frac{2}{3}}\bigr)$ and $C\beta_1^2\bigl(h_1^{-1}+h_1^{-\frac{2}{3}}\nu_1^{\frac{2}{3}}\bigr)^2$ respectively.

(c_2) As $M\ge 2$ contributions of γ-element to expressions (28.6.26) and (28.6.27) do not exceed respectively $C\beta_1 h_1^{-1}\nu_1^{\frac{1}{2}}$ and $C\beta_1^2 h_1^{-2}\nu_1$.

In the final tally $\gamma=1$ in both cases (c_1) and (c_2).

(d) Then for $M=1$ contributions of $\bar\gamma$-element to expressions (28.6.26) and (28.6.27) do not exceed respectively (in comparison to what we have already) $C\beta_1 h_1^{-\frac{2}{3}}\nu_1^{\frac{2}{3}}$ and $C\beta_1^2 h_1^{-\frac{4}{3}}\nu_1^{\frac{4}{3}}$ with $\nu_1=(\kappa\beta)^{\frac{10}{9}}h_1^{\frac{4}{9}}\bar\gamma^{\frac{58}{27}}|\log h|^K$.

On the other hand, for $M\ge 2$ contributions of $\bar\gamma$-element to expressions (28.6.26) and (28.6.27) do not exceed respectively (in comparison to what we have already) $C\beta_1 h_1^{-\frac{3}{2}}$ and $C\beta_1^2 h_1^{-3}$.

Let us partially summarize what we got. Let $\kappa\beta h\gtrsim 1$. Then for $M=1$ the final results are $C\beta\bigl(h^{-1}+h^{-\frac{2}{9}}(\kappa\beta)^{\frac{8}{9}}|\log h|^K\bigr)$ and the same expression squared. On the other hand, for $M\ge 2$ the final results from all zones except $\{x\colon \gamma(x)\le C_0\bar\gamma\}$ are $C\beta h^{-\frac{1}{3}}(\kappa\beta)^{\frac{2}{3}}|\log h|^K$ and the same expression squared.

On the other hand, let $\kappa\beta h\lesssim 1$. Then for $M=1$ the final results do not exceed $C\beta\bigl(h^{-1}+h^{-\frac{10}{27}}(\kappa\beta)^{\frac{20}{27}}|\log h|^K\bigr)$ and the same expression squared.

28.7 Applications to the Ground State Energy

28.7.1 Preliminary Remarks

Recall that we are looking for

$$\langle \mathsf{H}\Psi,\Psi\rangle+\frac{1}{\alpha}\int |\partial A'|^2\,dx, \tag{28.7.1}$$

which should be minimized by $\Psi\in\mathfrak{H}$ and A'.

We know (see f.e. Subsection 25.2.1) that

$$\begin{aligned}\langle \mathsf{H}\Psi,\Psi\rangle \ge \operatorname{Tr}^-(H_{A,W+\lambda'})+\lambda' N+\frac{1}{2}\mathsf{D}(\rho_\Psi-\rho,\,\rho_\Psi-\rho)\\ -\frac{1}{2}\mathsf{D}(\rho,\,\rho)-C\int \rho_\Psi^{\frac{4}{3}}\,dx,\end{aligned}\tag{28.7.2}$$

where $W=V-|x|^{-1}*\rho$, V is a Coulomb potential of nuclei, ρ and $\lambda\le 0$ are arbitrary.

Therefore to derive an estimate from below for expression (28.7.1) we just need to pick up ρ and λ' but we cannot pick up A'. Let us select ρ and λ equal to Thomas-Fermi density $=\rho_B^{\mathsf{TF}}$ and chemical potential λ respectively (but if $N\approx Z$ it is beneficial to pick up $\lambda'=0$), add $\alpha^{-1}\int|\partial A'|^2\,dx$, and apply trace asymptotics without any need to consider N- or D-terms and we have an estimate from below which includes also “bonus term” $\frac{1}{2}\mathsf{D}(\rho_\Psi-\rho,\,\rho_\Psi-\rho)$ and is as good as a remainder estimate in the trace asymptotics rescaled–provided we estimate properly the last term in (28.7.2).

Thus here we are missing only estimate for $\int\rho_\Psi^{\frac{4}{3}}\,dx$ or more sophisticated estimate if we are interested in Dirac and Schwinger terms. We will prove in Appendix 28.A.2 that in the electrostatic inequality for near ground-state one can replace this term $-C\int\rho_\Psi^{\frac{4}{3}}\,dx$ by $-CZ^{\frac{5}{3}}$ for $B\le Z^{\frac{4}{3}}$ and $-CB^{\frac{4}{5}}Z^{\frac{3}{5}}$ for $Z^{\frac{4}{3}}\le B\le Z^3$; further, for $B\le Z$ one can replace it by $\mathsf{Dirac}-CZ^{\frac{5}{3}-\delta}$ thus proving Bach-Graf-Solovej estimate in our current settings.

Therefore due to these arguments estimates from below in Theorems 28.7.4 and 28.7.5 follow immediately from Theorems 28.5.14, 28.5.16 and 28.5.23 for $B\le Z^{\frac{4}{3}}$ and estimates from below in Theorem 28.7.11 follow immediately from Theorems 28.6.2 and 28.6.4 for $Z^{\frac{4}{3}}\le B\le Z^3$.

On the other hand, an estimate from above involves picking up ρ (which we select to be ρ_B^{TF} again) and picking A' as well–which we choose as in upper estimates of Section 28.5 (rescaled) and also picking up Ψ which we select $\phi_1(x_1,\varsigma_1)\cdots\phi_N(x_N,\varsigma_N)$ anti-symmetrized by $(x_1,\varsigma_1),\dots,(x_N,\varsigma_N)$ but we do not select λ' in the trace asymptotics which *must* be equal to λ_N, which is N-th eigenvalue of $H_{W,A}$ or to 0 if there are less than N negative eigenvalues of $H_{W,A}$.

In this case we need to estimate $|\lambda'-\lambda|$ and also

$$\mathsf{D}\bigl(\operatorname{tr}e(x,x,\lambda')-\rho_B^{\mathsf{TF}},\,\operatorname{tr}e(x,x,\lambda')-\rho_B^{\mathsf{TF}}\bigr),\tag{28.7.3}$$

which required some efforts in Chapters 25–27 but here we will do it rather easily because in Section 28.5 we took either A' equal to one for Coulomb potential and without external magnetic field (as $\beta h^2 \le 1$) or just 0 (as $\beta h^2 \ge 1$).

28.7.2 Estimate from above: $B \le Z^{\frac{4}{3}}$

Recall that now we can select ρ and A' but cannot select λ'.

If $B \le Z^{\frac{4}{3}}$ (or $\beta h \le 1$ after rescaling) we select A' as a minimizer for one-particle operator with Coulomb potential and without external magnetic field. Then after rescaling $x \mapsto Z^{\frac{1}{3}} x$, $\tau \mapsto Z^{-\frac{4}{3}}\tau$, $h = 1 \mapsto h = Z^{-\frac{1}{3}}$, $B \mapsto \beta = BZ^{-1}$, $\alpha \mapsto \kappa = \alpha Z$

$$|\partial A'| \le C\kappa \ell^{-\frac{3}{2}}, \qquad |\partial^2 A'| \le C\kappa\ell^{-\frac{5}{2}} |\log(\ell/h^2)|, \tag{28.7.4}$$

or before it

$$|\partial A'| \le C\alpha Z^{\frac{5}{3}} \ell^{-\frac{3}{2}}, \qquad |\partial^2 A'| \le C\alpha Z^{\frac{5}{3}}\ell^{-\frac{5}{2}} |\log(Z\ell)|. \tag{28.7.5}$$

Let us start from the easy case $M = 1$. We need the following

Proposition 28.7.1. *Let $M = 1$, $N \asymp Z$, $B \lesssim Z^{\frac{4}{3}}$ and $\alpha Z \le \kappa^*$. Assume that A' satisfies* (28.7.5). *Then*

(i) The remainder in the trace asymptotics does not exceed

$$\begin{cases} C\bigl(Z^{\frac{5}{3}} + \alpha|\log(\alpha Z)|^{\frac{1}{3}} Z^{\frac{25}{9}}\bigr) & \text{for } B \le Z,\\ C\bigl(B^{\frac{1}{3}} Z^{\frac{4}{3}} + \alpha|\log(\alpha Z)|^{\frac{1}{3}} B^{\frac{2}{9}} Z^{\frac{23}{9}}\bigr) & \text{for } B \ge Z. \end{cases} \tag{28.7.6}$$

(ii) The remainder in N*-term asymptotics does not exceed* $CZ^{\frac{2}{3}}$.

(iii) D*-term does not exceed* $CZ^{\frac{5}{3}}$.

Proof. We cannot directly apply previous results because A' is now generated by much slower decaying Coulomb potential. The good news however is that A' is generated without presence of the external magnetic field. Let us scale as we mentioned above.

(i) Consider the remainder estimate in the trace asymptotics.

(ia) A contribution of the near singularity zone $\{x\colon \ell(x)\le \ell^*=\epsilon\min(\beta^{-\frac{2}{3}},1)\}$ does not exceed

$$\begin{cases} C(h^{-1}+\kappa|\log\kappa|^{\frac{1}{3}}h^{-\frac{4}{3}}) & \text{as}\quad \beta\le 1,\\ C(\beta^{\frac{1}{3}}h^{-1}+\kappa|\log\kappa|^{\frac{1}{3}}\beta^{\frac{2}{9}}h^{-\frac{4}{3}}) & \text{as}\quad \beta\ge 1.\end{cases}\tag{28.7.7}$$

(ib) A contribution of ℓ-element in the regular zone $\{x\colon \ell(x)\ge\ell^*\}$ does not exceed $C\zeta^2\bigl(h_1^{-1}+h_1^{-\frac{1}{3}}\nu_1^{\frac{2}{3}}\bigr)$. We plug $h_1=h/(\zeta\ell)$, and in virtue of (28.7.4) $\nu_1=\kappa\ell^{-\frac{5}{2}}\cdot\ell^3\zeta^{-1}=\kappa\ell^{\frac{1}{2}}\zeta^{-1}$. Taking a sum we arrive to the same expression at $\ell=\ell^*$ i.e. expression (28.7.7). Scaling back we arrive to (28.7.6).

(ic) We leave analysis of the boundary zone to the reader. It requires just repetition of the corresponding arguments of Section 28.5.

(ii) Next let us consider a remainder estimate in the N-term asymptotics.

(iia) Note that a contribution of ℓ-element in the regular zone does not exceed $C\bigl(h_1^{-2}+h_1^{-\frac{5}{3}}\nu_1^{\frac{1}{3}}\bigr)$. Then plugging h_1, ν_1 we arrive after summation to the same expression at $\ell=1$ i.e. Ch^{-2}. One can prove easily that the contribution of the near singularity zone is $O(h^{-2+\delta})$.

Consider the contribution of the boundary zone. Note that this zone appears only if $B\ge(Z-N)_+^{\frac{4}{3}}$. Let us scale $x\mapsto x\bar\ell^{-1}$, $\tau\mapsto\bar\ell^{-4}\tau$, with $\bar\ell=(\beta h)^{-\frac{1}{4}}$. Then $h\mapsto h_1=h^{\frac{3}{4}}\beta^{-\frac{1}{4}}$, $\beta\mapsto\beta_1=h_1^{-1}$ and after scaling A' satisfies $|\partial^2A'|\le\nu_1=C\kappa\bar\ell^{\frac{3}{2}}|\log\kappa|$.

(iib) Consider a contribution of γ-element; scaling again $x\mapsto x\gamma^{-1}$, $\tau\mapsto\gamma^{-4}\tau$, $h_1\mapsto h_2=h_1\gamma^{-3}$, $\beta_1\mapsto\beta\gamma^{-1}$, $\nu_1\mapsto\nu_2=\nu_1$ we see that it does not exceed $C\beta_2\bigl(h_2^{-1}+h_2^{-\frac{2}{3}}\nu_2^{\frac{2}{3}}\bigr)=C\beta_1\bigl(\gamma^2h_1^{-1}+\gamma h_1^{-\frac{2}{3}}\nu_1^{\frac{2}{3}}\bigr)$. This expression must be divided by γ^2 and summed resulting in

$$C\bigl(h_1^{-2}|\log\bar\gamma|+\bar\gamma^{-1}h_1^{-\frac{5}{3}}\nu_1^{\frac{2}{3}}\bigr)\tag{28.7.8}$$

with $\bar\gamma\ge h_1^{\frac{1}{3}}$ (equality is achieved if $(Z-N)_+$ is small enough, otherwise partitioning may be cut-off by a chemical potential). One can get rid of the logarithmic factor by our standard propagation arguments; the second term in (28.7.8) does not exceed $Ch_1^{-2}\nu_1^{\frac{2}{3}}$ and plugging h_1, ν_1 we get $O(h^{-2})=O(Z^{\frac{2}{3}})$.

(iii) D-term is analyzed in the same way. □

Proposition 28.7.2. *In the framework of Proposition 28.7.1 assume that* $B \le Z$. *Then*

(i) The remainder in the trace asymptotics (with the Schwinger term) does not exceed

$$CZ^{\frac{5}{3}}\bigl(Z^{-\delta} + (BZ^{-1})^{\delta}\bigr) + \alpha|\log(\alpha Z)|^{\frac{1}{3}}Z^{\frac{25}{9}}. \tag{28.7.9}$$

(ii) The remainder in N*-term asymptotics does not exceed* $CZ^{\frac{2}{3}}\bigl(Z^{-\delta} + (BZ^{-1})^{\delta} + (\alpha Z)^{\delta}\bigr)$.

(iii) D*-term does not exceed* $CZ^{\frac{5}{3}}\bigl(Z^{-\delta} + (BZ^{-1})^{\delta} + (\alpha Z)^{\delta}\bigr)$.

Proof. Proof includes improved (due to the standard arguments of propagation of singularities) estimates of the contributions of *threshold zone* $\{x\colon h^{\delta'} \le \ell(x) \le h^{-\delta'}\}$ after rescaling. We leave details to the reader. □

Since we now have exactly the same N-term asymptotics and the same remainder term estimate as in Subsection 26.6.3 as if there was no self-generated magnetic field we immediately arrive to the same estimates of $|\lambda_N - \lambda|$ as there and therefore to the same estimates for $|\lambda_N - \lambda|\cdot N$ and not only for two D-terms

$$\mathsf{D}\bigl(\operatorname{tr} e(x,x,\tau) - P'_B(W+\tau),\, \operatorname{tr} e(x,x,\tau) - P'_B(W+\tau)\bigr)$$

with $\tau = \lambda$ and $\tau = \lambda_N$ but also for the third one

$$\mathsf{D}\bigl(P'_B(W+\lambda_N) - P'_B(W+\lambda),\, P'_B(W+\lambda_N) - P'_B(W+\lambda)\bigr).$$

The trace term however is different–with Scott correction term $2S(\alpha Z)Z^2$ instead of $2S(0)Z^2$ and the remainder estimate here includes an extra term related to α.

It concludes the proof of the estimate from above for E^*_N. Combined with estimate from below it concludes the proof of Theorem 28.7.4.

Consider now the case $M \ge 2$. Since we need to decouple singularities in this case we need sufficiently fast decaying magnetic field and thus potential generating it. So we will take $A' = \sum_m A'_m\phi_m$ with A'_m defined by $V = W^{\mathsf{TF}}_m$

(where $\mathsf{W}_m^{\mathsf{TF}}$ corresponds to a single nucleus) without any magnetic field and with $N = Z$ (i.e. $\lambda = 0$) and ϕ_m is supported in $\{x\colon |x - \mathsf{y}_m \le \frac{1}{3}d\}$ and equals 1 in $\{x\colon |x - \mathsf{y}_m \le \frac{1}{4}d\}$. However everywhere else we take $V = W_B^{\mathsf{TF}}$.

Assume first that $(Z - N)_+$ is sufficiently small and we take $Z = N$ even in the definition of W_B^{TF}. Then one can prove easily that

$$|\operatorname{Tr}^-(H_{A,V}) + \alpha^{-1}\int |\partial A'|^2\,dx + \int P_B(V)\,dx - \mathsf{Scott}| \\ \le (28.7.6) + C\alpha Z^2 d^{-3}, \tag{28.7.10}$$

where the last term is due to decoupling; indeed, $|\partial A'|$ and $|\partial^2 A'|$ decay as ℓ^{-3} and ℓ^{-4} if $\ell \ge Z^{-\frac{1}{3}}$.

Moreover, for $B \le Z$ one can replace (28.7.6) by

$$CZ^{\frac{5}{3}}\bigl(Z^{-\delta} + (BZ^{-1})^{\delta} + (\alpha Z)^{\delta} + (dZ^{\frac{1}{3}})^{-\delta}\bigr) + C\alpha|\log(\alpha Z)|^{\frac{1}{3}} Z^{\frac{25}{9}} \tag{28.7.11}$$

while including $\mathsf{Schwinger}$ into left-hand expression. This estimate is at least as good as what we got in the estimate from below but probably even better since magnetic field admits now better estimates.

Let us estimate $|\lambda_N|$ if $\lambda_N < 0$. To do this consider

$$\int \bigl[e(x,x,\lambda) - e(x,x,\lambda_N)\bigr]\,dx \tag{28.7.12}$$

with non-negative integrand. Then the contribution of ℓ-element into the main part of this expression, namely

$$\int \bigl[e(x,x,\lambda) - e(x,x,\lambda_N)\bigr]\psi_\iota^2\,dx \tag{28.7.13}$$

is

$$\int \bigl[P'(x, V(x) + \lambda) - P'(x, V(x) + \lambda_N)\bigr]\psi_\iota^2\,dx \tag{28.7.14}$$

and it does not depend on A'. On the other hand, since now $|\partial^2 A'|$ admits so good estimate, the contribution of this element to the remainder estimated as if there was no self-generated magnetic field.

The same is true for the boundary elements as well.

But then $|\lambda_N|$ is estimated exactly as if there was no self-generated magnetic field, i.e. exactly as in Section 26.6. But then all components of the estimate from above, with exception of the trace term, namely $|\lambda_N|\cdot N$

and all three D-terms are estimated as in Section 26.6. Under assumption small $(Z-N)_+$ all of them do not exceed $CZ^{\frac{5}{3}}$ which could be improved to

$$CZ^{\frac{5}{3}}\bigl(Z^{-\delta}+(BZ^{-1})^{\delta}+(\alpha Z)^{\delta}+(dZ^{\frac{1}{3}})^{-\delta}\bigr) \tag{28.7.15}$$

for $B\le Z$.

Similarly, if $(Z-N)_+$ is larger than the corresponding threshold, we need to consider two cases: $0>\lambda>\lambda_N$ and $0>\lambda_N>\lambda$ and estimate from below

$$\int \bigl(e(x,x,\lambda)-e(x,x,\lambda_N)\bigr)\psi_\iota^2\,dx \tag{28.7.16}$$

and

$$\int \bigl(e(x,x,\lambda_N)-e(x,x,\lambda)\bigr)\psi_\iota^2\,dx \tag{28.7.17}$$

respectively, leading to the estimate of $|\lambda_N-\lambda|$ and then $|\lambda_N-\lambda|\cdot N$ and all three D-terms and again here these terms are estimated as if there was no self-generating magnetic field.

This concludes the proof of Theorem 28.7.5.

Remark 28.7.3. For $M\ge 2$ one could be concerned about term coming from $C\beta h^{-\frac{1}{2}}$ in the trace term and $C\beta h^{-\frac{3}{2}}$ or its square in N- and D-terms but assuming that $d\lesssim \bar{r}$ we simply have $A'=0$ due to decoupling there and therefore apply theory of Chapter 25 without any modification.

28.7.3 Main Theorems: $B\le Z^{\frac{4}{3}}$

Ground State Energy Asymptotics

Theorem 28.7.4. *Let $M=1$, $N\asymp Z$, $B\le Z^{\frac{4}{3}}$ and $\alpha\le\kappa^* Z^{-1}$ with small constant κ^*. Then*

(i) If $B\le Z$, then

$$\mathsf{E}_N^* = \mathcal{E}_N^{\mathsf{TF}} + \mathsf{Scott} + O\Bigl(Z^{\frac{5}{3}} + \alpha|\log(\alpha Z)|^{\frac{1}{3}} Z^{\frac{25}{9}}\Bigr) \tag{28.7.18}$$

with $\mathsf{Scott}=2Z^2S(\alpha Z)$.

(ii) Moreover, if $B \ll Z$ *and* $\alpha|\log Z|^{\frac{1}{3}} \ll Z^{-\frac{10}{9}}$, *then this estimate could be improved to*

$$\mathsf{E}^*_N = \mathcal{E}^{\mathsf{TF}}_N + 2Z^2 S(\alpha Z) + \mathsf{Schwinger} + \mathsf{Dirac} + O\Bigl(Z^{\frac{5}{3}}\bigl[Z^{-\delta} + B^{\delta} Z^{-\delta}\bigr] + \alpha|\log(\alpha Z)|^{\frac{1}{3}} Z^{\frac{25}{9}}\Bigr). \tag{28.7.19}$$

(iii) If $Z \le B \le Z^{\frac{4}{3}}$, *then*

$$\mathsf{E}^*_N = \mathcal{E}^{\mathsf{TF}}_N + 2Z^2 S(\alpha Z) + O\Bigl(B^{\frac{1}{3}} Z^{\frac{4}{3}} + \alpha|\log(\alpha Z)|^{\frac{1}{3}} B^{\frac{2}{9}} Z^{\frac{23}{9}} + \alpha B Z^{\frac{5}{3}}\Bigr). \tag{28.7.20}$$

Theorem 28.7.5. *Let* $M \ge 2$, $N \asymp Z_1 \asymp Z_2 \asymp \dots \asymp Z_M$, $B \lesssim Z^{\frac{4}{3}}$. *Let* $\alpha \le \kappa^* Z^{-1}$, $d \ge Z^{-\frac{1}{3}}$ *be a minimal distance between nuclei capped by* $\bar{r} = \min\bigl(B^{-\frac{1}{4}}, (Z-N)_+^{-\frac{1}{3}}\bigr)$. *Then*

(i) If $B \le Z$, *then*

$$\mathsf{E}^*_N = \mathcal{E}^{\mathsf{TF}}_N + \mathsf{Scott} + O\Bigl(Z^{\frac{5}{3}} + \alpha\bigl[|\log(\alpha Z)|^{\frac{1}{3}} Z^{\frac{25}{9}} + Z^2 d^{-3}\bigr]\Bigr) \tag{28.7.21}$$

with $\mathsf{Scott} = 2\sum_{1\le m\le M} Z_m^2 S(\alpha Z_m)$ *and, moreover,*

$$\mathsf{E}^*_N = \mathcal{E}^{\mathsf{TF}}_N + \mathsf{Scott} + \mathsf{Schwinger} + \mathsf{Dirac} + O\Bigl(Z^{\frac{5}{3}}\bigl[Z^{-\delta} + (BZ^{-1})^{\delta} + (dZ^{\frac{1}{3}})^{-\delta}\bigr] + \alpha\bigl[|\log(\alpha Z)|^{\frac{1}{3}} Z^{\frac{25}{9}} + Z^2 d^{-3}\bigr]\Bigr). \tag{28.7.22}$$

(ii) If $B \ge Z$, $\alpha B \le Z^{\frac{17}{60}}|\log Z|^{-K}$ *and* $(Z-N)_+ \le B^{\frac{5}{12}}$, *then*

$$\mathsf{E}^*_N = \mathcal{E}^{\mathsf{TF}}_N + \mathsf{Scott} + O\Bigl(B^{\frac{1}{3}} Z^{\frac{4}{3}} + \alpha\bigl[|\log\alpha|^{\frac{1}{3}} B^{\frac{2}{9}} Z^{\frac{23}{9}} + BZ^{\frac{5}{3}} + Z^2 d^{-3}\bigr]\Bigr); \tag{28.7.23}$$

(iii) If $B \ge Z^{\frac{77}{60}}|\log Z|^{-K}$, $\alpha \ge B^{-1} Z^{\frac{17}{60}}|\log Z|^{-K}$, $(Z-N)_+ \le B^{\frac{5}{12}}$ *and* $d \ge \bar{d} = (\alpha B)^{\frac{40}{209}} Z^{-\frac{81}{209}}|\log Z|^{K}$, *then*

$$\mathsf{E}^*_N = \mathcal{E}^{\mathsf{TF}}_N + \mathsf{Scott} \quad O\Bigl(B^{\frac{1}{3}} Z^{\frac{4}{3}} + \alpha\bigl[|\log\alpha|^{\frac{1}{3}} B^{\frac{2}{9}} Z^{\frac{23}{9}} + BZ^{\frac{5}{3}} + (\alpha B)^{\frac{120}{209}} Z^{\frac{384}{209}} d^{-3}|\log Z|^{K}\bigr]\Bigr). \tag{28.7.24}$$

(iv) In any case

$$\mathsf{E}^*_N = \mathcal{E}^{\mathsf{TF}}_N + \mathsf{Scott}_0 + O\bigl(B^{\frac{1}{3}}Z^{\frac{4}{3}} + \alpha Z^3\bigr) \tag{28.7.25}$$

with $\mathsf{Scott}_0 = 2\sum_{1\le m\le M} Z_m^2 S(0)$.

Recall that in the free nuclei model excess energy is $\asymp d^{-7}$ (as $d \le \epsilon B^{-\frac{1}{4}}$) and therefore an error must be greater than ϵd^{-7}. One can see easily that $d \ge \min(Z^{-\frac{5}{21}}, B^{-\frac{1}{4}})$ if $B \le Z$ and then in estimates (28.7.21) and (28.7.22) the last terms (with d^{-3}) could be skipped.

On the other hand, in (28.7.23)–(28.7.25) we can either skip the last terms (with d^{-3}) or assume that $d \asymp B^{-\frac{1}{4}}$ and these terms should be calculated under this assumption and we arrive to

Theorem 28.7.6. *Let $M \ge 2$, $N \asymp Z_1 \asymp Z_2 \asymp \dots \asymp Z_M$, $B \lesssim Z^{\frac{4}{3}}$ and $(Z-N)_+ \lesssim B^{\frac{1}{2}}$. Consider a free nuclei model. Then*

(i) If $B \le Z$, then

$$\hat{\mathsf{E}}^*_N = \hat{\mathcal{E}}^{\mathsf{TF}}_N + \mathsf{Scott} + O\Bigl(Z^{\frac{5}{3}} + \alpha\bigl[|\log(\alpha Z)|^{\frac{1}{3}} Z^{\frac{25}{9}}\bigr]\Bigr) \tag{28.7.26}$$

and moreover

$$\hat{\mathsf{E}}^*_N = \hat{\mathcal{E}}^{\mathsf{TF}}_N + \mathsf{Scott} + \mathsf{Schwinger} + \mathsf{Dirac} \\ + O\Bigl(Z^{\frac{5}{3}}\bigl[Z^{-\delta} + (BZ^{-1})^{\delta}\bigr] + \alpha\bigl[|\log(\alpha Z)|^{\frac{1}{3}} Z^{\frac{25}{9}}\bigr]\Bigr). \tag{28.7.27}$$

(ii) If $B \ge Z$, $\alpha \le B^{-1}Z^{\frac{17}{60}}|\log Z|^{-K}$, then

$$\hat{\mathsf{E}}^*_N = \hat{\mathcal{E}}^{\mathsf{TF}}_N + \mathsf{Scott} + O\Bigl(B^{\frac{1}{3}}Z^{\frac{4}{3}} + \alpha\bigl[|\log\alpha|^{\frac{1}{3}} B^{\frac{2}{9}} Z^{\frac{23}{9}} + Z^2 B^{\frac{3}{4}}\bigr]\Bigr). \tag{28.7.28}$$

(iii) If $B \ge Z^{\frac{77}{60}}|\log Z|^{-K}$, $B^{-1}Z^{\frac{17}{60}}|\log h|^{-K} \le \alpha \le B^{-\frac{369}{160}} Z^{\frac{81}{40}} |\log Z|^{-K}$, then

$$\mathsf{E}^*_N = \mathcal{E}^{\mathsf{TF}}_N + \mathsf{Scott} \\ O\Bigl(B^{\frac{1}{3}}Z^{\frac{4}{3}} + \alpha\bigl[|\log\alpha|^{\frac{1}{3}} B^{\frac{2}{9}} Z^{\frac{23}{9}} + (\alpha B)^{\frac{120}{209}} Z^{\frac{384}{209}} B^{\frac{3}{4}} |\log Z|^{K}\bigr]\Bigr). \tag{28.7.29}$$

(iv) In any case

$$\hat{\mathsf{E}}^*_N = \hat{\mathcal{E}}^{\mathsf{TF}}_N + \mathsf{Scott}_0 + O\bigl(B^{\frac{1}{3}}Z^{\frac{4}{3}} + \alpha Z^3\bigr). \tag{28.7.30}$$

We leave to the reader the following

Problem 28.7.7. In the frameworks of fixed nuclei and free nuclei models consider the case $M \ge 2$, $B \ge Z$ and $(Z-N)_+ \ge B^{\frac{5}{12}}$. Use results of Sections 28.5 and 26.6. Recall that there are two cases: $B^{\frac{5}{12}} \le (Z-N)_+ \le B^{\frac{3}{4}}$ and $(Z-N)_+ \ge B^{\frac{3}{4}}$.

In particular find out for which B this assumption could be skipped without deterioration of the remainder estimates.

Ground State Density Asymptotics

Consider now asymptotics of ρ_Ψ. Apart of independent interest one needs them for estimate of excessive negative charge and estimate or asymptotics of the ionization energy.

Theorem 28.7.8. *Let $M=1$, $N \asymp Z$, $B \lesssim Z^{\frac{4}{3}}$ and $\alpha \le \kappa^* Z^{-1}$, with small constant κ^*. Then*

(i) If $B \le Z$, then

$$\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}},\, \rho_\Psi - \rho^{\mathsf{TF}}) = O\bigl(Z^{\frac{5}{3}}\bigr) \tag{28.7.31}$$

and moreover this estimate could be improved to

$$\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}},\, \rho_\Psi - \rho^{\mathsf{TF}}) = O\Bigl(Z^{\frac{5}{3}}\bigl[Z^{-\delta} + B^{\delta}Z^{-\delta} + (\alpha Z)^{\delta}\bigr]\Bigr); \tag{28.7.32}$$

(ii) If $Z \le B \le Z^{\frac{4}{3}}$, then

$$\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}},\, \rho_\Psi - \rho^{\mathsf{TF}}) = O\Bigl(Z^{\frac{5}{3}} + (\alpha B)^{\frac{40}{27}} Z^{\frac{101}{81}} |\log Z|^{K}\Bigr). \tag{28.7.33}$$

Proof. We need to consider only the case when errors in the estimates for E^*_N exceed those announced in (28.7.31)–(28.7.33). Otherwise an estimate for $\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}},\, \rho_\Psi - \rho^{\mathsf{TF}})$ follow from the estimates from above and below for E^*_N as estimates from below contain the "bonus term" $\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}},\, \rho_\Psi - \rho^{\mathsf{TF}})$.

Let in the estimate from below pick up $\lambda' = \lambda_N$ and in the estimate from above pick up A' as a minimizer for a potential $W^{\mathsf{TF}}_B + \lambda'$ with $\lambda' = \lambda_N$; we do not calculate asymptotics of the trace terms since these terms in both estimates coincide[36]; then we arrive to estimate

$$\mathsf{D}(\rho_\Psi-\rho^{\mathsf{TF}},\,\rho_\Psi-\rho^{\mathsf{TF}})\\ \le C\mathsf{D}(\operatorname{tr} e(x,x,\lambda_N)-\rho^{\mathsf{TF}},\,\operatorname{tr} e(x,x,\lambda_N)-\rho^{\mathsf{TF}})+CZ^{\frac{5}{3}} \tag{28.7.34}$$

and we need to estimate the first term in the right-hand expression.

Let us scale as usual. Then $\beta h\lesssim 1$ since $B\le Z^{\frac{4}{3}}$ and our standard arguments estimate this term by $C\bigl(h^{-2}+h^{-\frac{5}{3}}\nu^{\frac{2}{3}}\bigr)^2$ with $\nu=(\kappa\beta)^{\frac{10}{9}}h^{\frac{4}{9}}|\log h|^K$.

Plugging $\beta=BZ^{-1}$, $h=Z^{-\frac{1}{3}}$, $\kappa=\alpha Z$ and multiplying by $Z^{\frac{1}{3}}$ due to the spatial scaling we arrive exactly to (28.7.31) and (28.7.33).

Furthermore, as $\beta\ll 1$ let us consider contribution of the *main zone* $\{x\colon h^\delta\le \ell(x)\le h^{-\delta}+(\beta+\kappa)^\delta\}$ and use propagation arguments and improved electrostatic inequality; then we arrive to estimate $Ch^{-4}(h+\beta+\kappa)^\delta$ which after rescaling becomes (28.7.32).

We leave all easy details to the reader. □

Consider now case $M\ge 2$. Then no matter what is the distance between nuclei (as long as it is greater than $\epsilon Z^{-\frac{1}{3}}$) we need to add one or two more extra terms.

(a) The first one always appears and it is what becomes from $C\beta_1^2h_1^{-2}\nu_1\ell^{-1}$ as we plug $\beta_1=\beta\ell^3$, $h_1=h\ell$, $\kappa_1=\kappa\ell^{-3}$, $\nu_1=(\kappa_1\beta_1)^{\frac{10}{9}}h_1^{\frac{4}{9}}|\log h_1|^K\asymp(\kappa\beta)^{\frac{10}{9}}h^{\frac{4}{9}}\ell^{\frac{4}{9}}|\log h|^K$, and multiply by ℓ^{-1} we get ℓ in the positive power and therefore we must plug the largest possible ℓ which in case $(Z-N)_+\le B^{\frac{3}{4}}$ is $\ell=(\beta h)^{-\frac{1}{4}}$. Also plugging $\kappa=\alpha Z$, $\beta=BZ^{-1}$, $h=Z^{-\frac{1}{3}}$ and $\ell=(\beta h)^{-\frac{1}{4}}=B^{-\frac{1}{4}}Z^{\frac{1}{3}}$ and multiplying by $Z^{\frac{1}{3}}$ due to the scaling (with a possible improvement for $B\ll Z$) we arrive to $\alpha^{\frac{40}{27}}B^{\frac{9}{4}}|\log Z|^K$. One can see easily that this term is larger than the second term in (28.7.33).

For $(Z-N)_+\ge B^{\frac{3}{4}}$ this term will be smaller than the second extra term.

(b) The second extra term appears only if $(Z-N)_+\gtrsim B^{\frac{5}{12}}$.

(b)$_1$ For $B^{\frac{5}{12}}\le (Z-N)_+\le B^{\frac{3}{4}}$ it is what becomes from $\beta_2^2h_2^{-3}\bar\gamma^{-4}|\log\bar\gamma|^2$ with substitutions $\beta_2=\beta_1\bar\gamma^{-1}$, $h_2=h_1\bar\gamma^{-3}$, $\bar\gamma=(Z-N)_+^{\frac{1}{4}}B^{-\frac{3}{16}}$ and with β_1,h_1,ℓ defined above (we still need to multiply by $Z^{\frac{1}{3}}$).

[36] Due to the matching choices of A' and λ'.

(b)$_2$ For $(Z-N)_+\geq B^{\frac{3}{4}}$ it is what becomes out $\beta_1^2 h_1^{-3}\ell^{-1}$ with $\ell=(Z-N)_+^{-\frac{1}{3}}$.

Thus we arrive to

Theorem 28.7.9. *Let $M\geq 2$, $N\asymp Z_1\asymp \ldots\asymp Z_M$, $B\lesssim Z^{\frac{4}{3}}$. Further, let $\alpha\leq \kappa^* Z^{-1}$, $d\gtrsim Z^{-\frac{1}{3}}$. Then*

(i) For $B\leq Z$ estimate (28.7.31) *holds and, moreover, it could be improved to*

$$\mathsf{D}(\rho_\Psi-\rho^{\mathsf{TF}},\,\rho_\Psi-\rho^{\mathsf{TF}}) = O\Bigl(Z^{\frac{5}{3}}\bigl[Z^{-\delta}+B^\delta Z^{-\delta}+(\alpha Z)^\delta+(dZ^{\frac{1}{3}})^{-\delta}\bigr]\Bigr). \tag{28.7.35}$$

(ii) For $B\geq Z$ and $(Z-N)_+\leq B^{\frac{5}{12}}$

$$\mathsf{D}(\rho_\Psi-\rho^{\mathsf{TF}},\,\rho_\Psi-\rho^{\mathsf{TF}}) = O\Bigl(Z^{\frac{5}{3}}+\alpha^{\frac{10}{9}}B^{\frac{9}{4}}|\log Z|^K\Bigr). \tag{28.7.36}$$

(iii) For $B\geq Z$ and $B^{\frac{5}{12}}\leq (Z-N)_+\leq B^{\frac{3}{4}}$

$$\mathsf{D}(\rho_\Psi-\rho^{\mathsf{TF}},\,\rho_\Psi-\rho^{\mathsf{TF}}) = O\Bigl(Z^{\frac{5}{3}}+\alpha^{\frac{10}{9}}B^{\frac{9}{4}}|\log Z|^K + B^{\frac{15}{16}}(Z-N)_+^{\frac{3}{4}}(1+|\log (Z-N)_+B^{-\frac{1}{3}}|)^2\Bigr). \tag{28.7.37}$$

(iv) For $B\geq Z$ and $(Z-N)_+\leq B^{\frac{3}{4}}$

$$\mathsf{D}(\rho_\Psi-\rho^{\mathsf{TF}},\,\rho_\Psi-\rho^{\mathsf{TF}}) = O\Bigl(Z^{\frac{5}{3}}+B^2(Z-N)_+^{-\frac{2}{3}}\Bigr). \tag{28.7.38}$$

Corollary 28.7.10. *Estimates* (28.7.31), (28.7.35)– (28.7.38) *hold for a free nuclei model.*

28.7.4 Main Theorems: $Z^{\frac{4}{3}}\leq B\leq Z^3$

Ground State Energy Asymptotics

For $Z^{\frac{4}{3}}\leq B\leq Z^3$ we select $A'=0$ in the estimate from above and therefore just apply an upper estimate E_N^* from Subsection 26.6.3. Combined with estimate from below provided by Theorem 28.6.2 it implies the following

Theorem 28.7.11. *Let* $Z^{\frac{4}{3}} \lesssim B \lesssim Z^3$, $Z_1 \asymp ... \asymp Z_M \asymp N$, *and* $\alpha \le \kappa^* Z^{-1}$ *with small constant* κ^*, *and also* $\alpha \le B^{-\frac{4}{5}} Z^{\frac{2}{5}} |\log Z|^{-K}$. *Then*

(i) For $M=1$ *and either* $(Z-N)_+ \lesssim B^{\frac{4}{15}} Z^{\frac{1}{5}}$ *or* $\alpha B^{\frac{3}{5}} Z^{\frac{1}{5}} \gtrsim 1$

$$|\mathsf{E}^*_N - \mathcal{E}^{\mathsf{TF}}_N - \mathsf{Scott}_0| \tag{28.7.39}$$

does not exceed

$$C\Bigl(B^{\frac{1}{3}} Z^{\frac{4}{3}} + B^{\frac{4}{5}} Z^{\frac{3}{5}} + \alpha Z^3 + \alpha^{\frac{16}{9}} B^{\frac{82}{45}} Z^{\frac{49}{45}} |\log Z|^K\Bigr). \tag{28.6.3}$$

(ii) For $M=1$ *and* $(Z-N)_+ \gtrsim B^{\frac{4}{15}} Z^{\frac{1}{5}}$ *and* $\alpha B^{\frac{3}{5}} Z^{\frac{1}{5}} \lesssim 1$ *expression* (28.7.39) *does not exceed*

$$C\Bigl(B^{\frac{1}{3}} Z^{\frac{4}{3}} + B^{\frac{4}{5}} Z^{\frac{3}{5}} + \alpha Z^3 + \alpha^{\frac{16}{9}} B^{\frac{82}{45}} Z^{\frac{49}{45}} |\log Z|^K \\ + \alpha^{\frac{40}{27}} B^{\frac{13}{15}} Z^{\frac{139}{135}} (Z-N)_+^{\frac{28}{27}} |\log Z|^K\Bigr). \tag{28.6.4}$$

(iii) For $M \ge 2$ *and* $(Z-N)_+ \lesssim B^{\frac{4}{15}} Z^{\frac{1}{5}}$ *expression* (28.7.39) *does not exceed*

$$C\Bigl(B^{\frac{1}{3}} Z^{\frac{4}{3}} + B^{\frac{4}{5}} Z^{\frac{3}{5}} (1 + |\log BZ^{-3}|)^2 + \alpha Z^3 + \alpha^{\frac{16}{9}} B^{\frac{82}{45}} Z^{\frac{49}{45}} |\log Z|^K\Bigr). \tag{28.7.40}$$

(iv) For $M \ge 2$ *and* $(Z-N)_+ \gtrsim B^{\frac{4}{15}} Z^{\frac{1}{5}}$ *expression* (28.7.39) *does not exceed*

$$C\Bigl(B^{\frac{1}{3}} Z^{\frac{4}{3}} + B^{\frac{4}{5}} Z^{\frac{3}{5}} (1 + |\log BZ^{-3}|)^2 + \alpha Z^3 + \alpha^{\frac{16}{9}} B^{\frac{82}{45}} Z^{\frac{49}{45}} |\log Z|^K \\ + B^{\frac{2}{3}} (Z-N)_+ (1 + |\log (Z-N)_+ Z^{-1}|)^2\Bigr). \tag{28.7.41}$$

Ground State Density Asymptotics

Consider now asymptotics of ρ_Ψ. Apart of independent interest we need them for estimate of excessive negative charge and estimate or asymptotics of the ionization energy. We are interested as usual in $\mathsf{D}\bigl(\rho_\Psi - \rho_B^{\mathsf{TF}},\, \rho_\Psi - \rho_B^{\mathsf{TF}}\bigr)$ and we know that

Corollary 28.7.12. *In the framework of Theorem 28.7.11(i), (ii), (iii), (iv)* $\mathsf{D}\bigl(\rho_\Psi - \rho_B^{\mathsf{TF}},\, \rho_\Psi - \rho_B^{\mathsf{TF}}\bigr)$ *does not exceed the corresponding remainder estimate* (28.6.3), (28.6.4), (28.7.40), (28.7.41).

If we want to get rid of $\alpha Z^3 + B^{\frac{1}{3}}Z^{\frac{4}{3}}$ terms (which may be dominant only for $B \le Z^{\frac{7}{4}}$ and $B \le Z^{\frac{11}{7}}$ respectively) we need not to find asymptotics of the trace term but to have trace term in the estimates from above and below more consistent. The only explored option is to take in the estimate from above the same A' as in the estimate from below, which is a minimizer for the corresponding one particle problem.

Theorem 28.7.13. *Let $Z^{\frac{4}{3}} \lesssim B \lesssim Z^3$, $Z_1 \asymp ... \asymp Z_M \asymp N$, and $\alpha \le \kappa^* Z^{-1}$ with small constant κ^*, and also $\alpha \le B^{-\frac{4}{5}}Z^{\frac{2}{5}}|\log Z|^{-K}$.*

(i) Let $M=1$. Then $\mathsf{D}\bigl(\rho_\Psi - \rho_B^{\mathsf{TF}}, \rho_\Psi - \rho_B^{\mathsf{TF}}\bigr)$ does not exceed

$$CB^{\frac{4}{5}}Z^{\frac{3}{5}} + C\Bigl(\alpha^{\frac{16}{9}}B^{\frac{82}{45}}Z^{\frac{49}{45}} + \alpha^{\frac{40}{27}}B^{-\frac{10}{9}}Z^{\frac{127}{27}} + \alpha^{\frac{40}{27}}B^{\frac{74}{45}}Z^{\frac{11}{90}}(Z-N)_+^{\frac{29}{54}}\Bigr)|\log Z|^K. \tag{28.7.42}$$

(ii) Let $M=2$ and the minimal distance between nuclei $d \gtrsim B^{-\frac{2}{5}}Z^{\frac{1}{5}}$. Then $\mathsf{D}\bigl(\rho_\Psi - \rho_B^{\mathsf{TF}}, \rho_\Psi - \rho_B^{\mathsf{TF}}\bigr)$ does not exceed

$$CB^{\frac{4}{5}}Z^{\frac{3}{5}} + C\Bigl(\alpha^{\frac{4}{3}}B^{\frac{22}{15}}Z^{\frac{19}{15}} + \alpha^{\frac{40}{27}}B^{-\frac{10}{9}}Z^{\frac{127}{27}} + B^{\frac{3}{5}}Z^{\frac{9}{20}}(Z-N)_+^{\frac{3}{4}}\Bigr)|\log Z|^K. \tag{28.7.43}$$

Proof. We will use Propositions 28.6.5 and 28.6.6 to estimate (28.6.27). Let us consider for each partition element

$$|\int \bigl(e(x,x,\lambda') - P_B(V(x)+\lambda')\bigr)\psi(x)\,dx|. \tag{28.7.44}$$

(a) Zone $\{x\colon \ell(x) \le B^{-1}Z|\log h|^\delta\}$. Here for each ℓ-element expression (28.7.44) does not exceed $R_a = C(h_1^{-2} + \beta_1 h_1^{-1})(1 + \nu_1^{\frac{2}{3}}h_1^{\frac{1}{3}})$ with $\beta_1 = \beta\ell^{\frac{3}{2}}$, $h_1 = h\ell^{-\frac{1}{2}}$ and ν_1 defined according to Proposition 28.6.5(ii). As usual $\beta = B^{\frac{2}{5}}Z^{-\frac{1}{5}}$ and $h = B^{\frac{1}{5}}Z^{-\frac{3}{5}}$.

Then one can prove easily that the total contribution of this zone to

$$\mathsf{D}\bigl(e(x,x,\lambda') - P_B(V(x)+\lambda'),\, e(x,x,\lambda') - P_B(V(x)+\lambda')\bigr) \tag{28.7.45}$$

does not exceed $CBZ^{-1}R_a^2$ [37] which is the second term in the parenthesis of (28.7.42) and (28.7.43) [38].

(b) Zone $\{x\colon B^{-1}Z|\log h|^\delta \le \ell(x) \le \epsilon B^{-\frac{2}{5}}Z^{\frac{1}{5}}\}$ (with the exception of the case $\bar\gamma \ge |\log h|^{-\delta}$ which we leave to the reader). Here for each ℓ-element expression (28.7.44) does not exceed $R_b = C\beta_1 h_1^{-1}(1+\nu_1^{\frac{2}{3}}h_1^{\frac{1}{3}})$ with $\beta_1=\beta\ell^{\frac{3}{2}}$, $h_1 = h\ell^{-\frac{1}{2}}$ and ν_1 defined according to Proposition 28.6.6(i).

Then one can prove easily that the total contribution of this zone to (28.7.45) does not exceed $CB^{\frac{2}{5}}Z^{-\frac{1}{5}}R_b^2$ [37] which is the first term in the parenthesis of (28.7.42) [38].

(c) Zone $\{x\colon \bar\gamma|\log h|^\delta \le \gamma(x) \le C_0\}$. Here for each γ-element expression (28.7.44) does not exceed R_c where $R_c = C\beta_2 h_2^{-1}(1+\nu_2^{\frac{2}{3}}h_2^{\frac{1}{3}})$ (as $M=1$) and $R_c = C\beta_2 h_2^{-1}\nu_2^{\frac{1}{2}}$ (as $M\ge 2$) with $\beta_2=\beta\gamma^{-1}$, $h_2 = h\gamma^{-3}$ and ν_2 defined by Proposition 28.6.6(i) and redefined by Remark 28.5.9.

Then one can prove easily that the total contribution of this zone to (28.7.45) does not exceed $CB^{\frac{2}{5}}Z^{-\frac{1}{5}}R_c^2$ [37] which is the first term in the parenthesis of (28.7.42) and (28.7.43) for $M=1$ and $M\ge 2$ respectively [38].

(d) Zone $\{x\colon \gamma(x)\le \bar\gamma|\log h|^\delta\}$. Here for each γ-element expression (28.7.44) does not exceed $R_d = C\beta_2 h_2^{-1}(1+\nu_2^{\frac{2}{3}}h_2^{\frac{1}{3}})$ (as $M=1$) and $R_d = C\beta_2 h_2^{-\frac{3}{2}}$ (as $M\ge 2$) with $\beta_2=\beta\gamma^{-1}$, $h_2=h\gamma^{-3}$ and ν_2 defined by Proposition 28.6.6(ii).

Then one can prove easily that the total contribution of this zone to (28.7.45) does not exceed $CB^{\frac{2}{5}}Z^{-\frac{1}{5}}R_d^2\bar\gamma^{-4}$ [37] which is the third term in the parenthesis of (28.7.42) and (28.7.43) for $M=1$ and $M\ge 2$ respectively [38]. $\square$

28.A Appendices

28.A.1 Generalization of Lieb-Loss-Solovej Estimate

Proposition 28.A.1. *Consider operator H defined by* (27.1.1) *with* $A = A'+A''$, $A'=(A'_1(x'),A'_2(x'),0)$, $x'=(x_1,x_2)$, *and* $A''=(A''_1(x),A''_2(x),A''_3(x))$

[37] Calculated for ℓ or γ on its maximum.

[38] Modulo term not exceeding $CB^{\frac{4}{5}}Z^{\frac{3}{5}}$.

on Ω. *Assume that*

$$\int B'^2\,dx \ge \int B''^2\,dx \tag{28.A.1}$$

with $B=|\nabla\times A|$, $B'=|\nabla\times A'|$, $B''=|\nabla\times A''|$. *Then*

$$\begin{multline} -\operatorname{Tr}(H^-_{A,V})\le \\ C\int V_+^{\frac{5}{2}}(x)\,dx + C\Bigl(\int B^2\,dx\Bigr)^{\frac12}\Bigl(\int B''^2\,dx+\int V^2\,dx\Bigr)^{\frac14}\Bigl(\int V^4\,dx\Bigr)^{\frac14}+\\ C\Bigl(\int B^2\,dx\Bigr)^{\frac38}\Bigl(\int V^2\,dx\Bigr)^{\frac38}\Bigl(\int V^4\,dx\Bigr)^{\frac14}. \end{multline} \tag{28.A.2}$$

Proof. Without any loss of the generality we can assume that $V\ge 0$. We apply the *moving frame technique* of Lieb-Loss-Solovej [1]. Obviously

$$\begin{multline} -\operatorname{Tr}(H^-_{A,V})=\int_0^\infty \mathsf{N}^-(H_{A,V}+\lambda)\,d\lambda=\\ \int_0^\infty \mathsf{N}^-(H_{A,0}+\lambda-V)\,d\lambda\le \int_0^\infty \mathsf{N}^-\bigl(H_{A,0}+(\lambda-V)\phi(\lambda)\bigr)\,d\lambda \end{multline} \tag{28.A.3}$$

with $\phi(\lambda)=\max(1,\lambda\mu^{-1})$ since $H_{A,0}\ge 0$. Since

$$\begin{multline} H_{A,0}=\bigl(P\cdot\boldsymbol{\sigma}\bigr)^2=\bigl(P'\cdot\boldsymbol{\sigma}'\bigr)^2+P_3^2+\sum_{j=1,2}[P_j,P_3]\,[\sigma_j,\sigma_3]\ge\\ H'_{A,0}+P_3^2-B'' \end{multline} \tag{28.A.4}$$

with

$$H'_{A,0}=\bigl(P'\cdot\boldsymbol{\sigma}'\bigr)^2=\bigl(\sum_{j=1,2}P_j\cdot\sigma_j\bigr)^2, \tag{28.A.5}$$

$P_j=D_j-A_j$, we conclude that $-\operatorname{Tr}(H^-_{A,V})$ does not exceed

$$\int_0^\infty \mathsf{N}^-\bigl(H'_{A,0}+P_3^2-B''+(\lambda-V)\phi(\lambda)\bigr)\,d\lambda. \tag{28.A.6}$$

Consider this integral over (μ,∞); it is equal to

$$\int_\mu^\infty \mathsf{N}^-\bigl(H'_{A,0}+P_3^2-B''+(\lambda-V)\lambda\mu^{-1}\bigr)\,d\lambda \tag{28.A.7}$$

and since $H'_{A,0}\ge 0$ this integral does not exceed

$$\int_\mu^\infty \mathsf{N}^-\bigl(H'_{A,0}+a[P_3^2-B''+(\lambda-V)\lambda\mu^{-1}]\bigr)\,d\lambda \tag{28.A.8}$$

with $a\ge 1$; since $H'_{A,0}\ge P_1^2+P_2^2-|B|$ this integral (28.A.8) does not exceed

$$\int_\mu^\infty \mathsf{N}^-\bigl(P_1^2+P_2^2-B+a[P_3^2-B''+(\lambda-V)\lambda\mu^{-1}]\bigr)\,d\lambda \tag{28.A.9}$$

which can be estimated due to CLR inequality after rescaling $x_3\mapsto a^{\frac{1}{2}}x_3$, $P_3\mapsto a^{-\frac{1}{2}}P_3$ by

$$\begin{aligned}C\int\int_\mu^\infty a^{-\frac{1}{2}}\bigl(B+a[B''+(V-\lambda)\lambda\mu^{-1}]\bigr)_+^{\frac{3}{2}}\,d\lambda dx\\
\le C\int\int_\mu^\infty a^{-\frac{1}{2}}\bigl(B-\frac{1}{3}a\lambda^2\mu^{-1}\bigr)_+^{\frac{3}{2}}\,d\lambda dx\\
+C\int\int_\mu^\infty a\bigl(B''-\frac{1}{3}\lambda^2\mu^{-1}\bigr)_+^{\frac{3}{2}}\,d\lambda dx\\
+C\int\int_\mu^\infty a(\lambda\mu^{-1})^{\frac{3}{2}}(V-\frac{1}{3}\lambda)_+^{\frac{3}{2}}\,d\lambda dx\\
\le Ca^{-1}\mu^{\frac{1}{2}}\int B^2\,dx+Ca\mu^{\frac{1}{2}}\int B''^2\,dx+Ca\mu^{-\frac{3}{2}}\int V^4\,dx,\end{aligned}$$

where we integrated over $[0,\infty]$. Optimizing with respect to $a\ge 1$ we get

$$\begin{aligned}C\Bigl(\int B^2\,dx\Bigr)^{\frac{1}{2}}\Bigl(\mu\int B''^2\,dx+\mu^{-1}\int V^4\,dx\Bigr)^{\frac{1}{2}}\\
+C\mu^{\frac{1}{2}}\int B''^2\,dx+C\mu^{-\frac{3}{2}}\int V^4\,dx.\end{aligned}\tag{28.A.10}$$

Therefore integral (28.A.7) does not exceed (28.A.10).

Consider integral (28.A.6) over $[0,\mu]$; it is

$$\int_0^\mu \mathsf{N}^-\bigl(H'_{A,0}+P_3^2-B''+(\lambda-V)\bigr)\,d\lambda \tag{28.A.11}$$

and exactly as before it does not exceed

$$\begin{aligned}C\int\int_0^\mu a^{-\frac{1}{2}}\bigl(B-\frac{1}{3}a\lambda\bigr)_+^{\frac{3}{2}}\,d\lambda dx+C\int\int_0^\mu a\bigl(B''-\frac{1}{3}\lambda\bigr)_+^{\frac{3}{2}}\,d\lambda dx\\
+C\int\int_0^\mu a(V-\frac{1}{3}\lambda)_+^{\frac{3}{2}}\,d\lambda dx\end{aligned}$$

with $a \geq 1$; in first two integrals we replace (in parenthesis) λ by $\lambda^2\mu^{-1}$ and expand integral to $[0,\infty]$, arriving to

$$Ca^{-1}\mu^{\frac{1}{2}}\int B^2\,dx + Ca\mu^{\frac{1}{2}}\int B''^2\,dx + C\int aV^{\frac{3}{2}}\min(V,\mu)\,dx;$$

optimizing with respect to $a \geq 1$ we get

$$C\Bigl(\int B^2\,dx\Bigr)^{\frac{1}{2}}\Bigl(\mu\int B''^2\,dx + \mu^{\frac{1}{2}}\int V^{\frac{3}{2}}\min(V,\mu)\,dx\Bigr)^{\frac{1}{2}} + C\mu^{\frac{1}{2}}\int B''^2\,dx + C\int V^{\frac{3}{2}}\min(V,\mu)\,dx. \tag{28.A.12}$$

Therefore integral (28.A.11) does not exceed (28.A.12) and the whole expression does not exceed

$$C\Bigl(\int B^2\,dx\Bigr)^{\frac{1}{2}}\Bigl(\mu\int B''^2\,dx + \mu^{-1}\int V^4\,dx + \mu^{\frac{1}{2}}\int V^{\frac{3}{2}}\min(V,\mu)\,dx\Bigr)^{\frac{1}{2}} + C\mu^{\frac{1}{2}}\int B''^2\,dx + C\mu^{-\frac{3}{2}}\int V^4\,dx + C\int V^{\frac{3}{2}}\min(V,\mu)\,dx;$$

replacing $\min(V,\mu)$ by $V^{\frac{1}{2}}\mu^{\frac{1}{2}}$ and V in the first and second lines respectively we get

$$C\Bigl(\int B^2\,dx\Bigr)^{\frac{1}{2}}\Bigl(\mu\int B''^2\,dx + \mu^{-1}\int V^4\,dx + \underline{\mu\int V^2\,dx}\Bigr)^{\frac{1}{2}} + C\mu^{\frac{1}{2}}\int B''^2\,dx + C\mu^{-\frac{3}{2}}\int V^4\,dx + C\int V^{\frac{5}{2}}\,dx.$$

We skip the last term since it is already in (28.A.2); temporarily skip monotone increasing by μ selected term; optimizing the rest by $\mu > 0$ we get

$$C\Bigl(\int B^2\,dx\Bigr)^{\frac{1}{2}}\Bigl(\int B''^2\,dx\Bigr)^{\frac{1}{4}}\Bigl(\int V^4\,dx\Bigr)^{\frac{1}{4}}.$$

Now we are left with

$$C\mu^{\frac{1}{2}}\Bigl(\int B^2\,dx\Bigr)^{\frac{1}{2}}\Bigl(\int V^2\,dx\Bigr)^{\frac{1}{2}} + C\mu^{-\frac{1}{2}}\Bigl(\int B^2\,dx\Bigr)^{\frac{1}{2}}\Bigl(\int V^4\,dx\Bigr)^{\frac{1}{2}} + C\mu^{-\frac{3}{2}}\int V^4\,dx.$$

Optimizing by $\mu > 0$ we get

$$C\Bigl(\int B^2\,dx\Bigr)^{\frac{1}{2}}\Bigl(\int V^2\,dx\Bigr)^{\frac{1}{4}}\Bigl(\int V^4\,dx\Bigr)^{\frac{1}{4}}+ \\ C\Bigl(\int B^2\,dx\Bigr)^{\frac{3}{8}}\Bigl(\int V^2\,dx\Bigr)^{\frac{3}{8}}\Bigl(\int V^4\,dx\Bigr)^{\frac{1}{4}}$$

which concludes the proof. □

28.A.2 Electrostatic Inequality

Proposition 28.A.2. *(i) Let $B \le Z^3$, $\alpha \le \kappa^* Z^{-1}$, $c^{-1}Z \le N \le cZ$. Further, if $B \ge Z^{\frac{4}{3}}$ then $\alpha B^{\frac{4}{5}} Z^{-\frac{2}{5}} \le \epsilon$. Then*

$$\sum_{1\le j<k\le M} \int |x_j - x_k|^{-1} |\Psi(x_1,\dots,x_N)|^2\, s dx_1\cdots dx_N \\ \ge \mathsf{D}(\rho_\Psi,\rho_\Psi) - C\bigl(Z^{\frac{5}{3}} + B^{\frac{2}{5}} Z^{\frac{17}{15}} + B\bigr); \tag{28.A.13}$$

(ii) Further, afor $B \le Z$ one can replace the last term in (28.A.13) *by* $\mathsf{Dirac} - CZ^{\frac{5}{3}-\delta}$.

Remark 28.A.3. Without self-generated magnetic field the last term was $-C(Z^{\frac{5}{3}} + B^{\frac{2}{5}} Z^{\frac{17}{15}})$ and probably it holds here but does not give us any advantage; for $B \ge Z$ we need only $C\bigl(Z^{\frac{5}{3}} + B^{\frac{4}{5}} Z^{\frac{3}{5}}\bigr)$ estimate.

Proof. Since we prove estimate from below we replace first

$$\langle \sum_{1\le j\le N} (H_{A,V})_{x_j}\Psi,\, \Psi\rangle$$

by

$$\langle \sum_{1\le j\le N} (H_{A,W})_{x_j}\Psi,\, \Psi\rangle + \int (W-V)\rho_\Psi\,dx$$

without changing anything else and then we estimate the first term here from below by $\mathsf{Tr}(H^-_{A,W})$; then in $\mathsf{Tr}(H^-_{A,W}) + \alpha^{-1}\|\partial A'\|^2$ we replace A' by a minimizer for this expression (rather than for the original problem) only decreasing this expression. So we can now consider A' a minimizer of Section 28.5.

Then we follow arguments of Appendix 26.A.1 but now we need to justify magnetic Lieb-Thirring estimate (26.A.12)

$$\mathsf{Tr}(H^-_{A,W}) \ge -C\int P_B(W)\,dx \tag{26.A.12}$$

in the current settings and with $W : CP'(W) = \rho_\Psi$ and then $W \asymp \min(B^{-2}\rho_\Psi^2; \rho_\Psi^{\frac{2}{3}})$.

Estimate (26.A.12) has been proven in L. Erdös [1] (Theorem 2.2) under assumption that intensity of the magnetic field $\vec{B}(x)$ has a constant direction which was the case in Chapter 25 but not here.

However we actually we do not need (26.A.12); we need this estimate but with an extra term $-CR$ in the right-hand expression where in (i) $R = (Z^{\frac{5}{3}} + B^{\frac{4}{5}}Z^{\frac{3}{5}})$ is the last term in (28.A.13) and in (ii) $R = CZ^{\frac{5}{3}-\delta}$.

Further, the same paper L. Erdös [1]) provides an alternative version of Theorem 2.2: as long as $|\partial A'| \le B$ it is sufficient to estimate $|\partial^2 A| \le cB^{\frac{3}{2}}$.

One can check easily that this pointwise estimate holds if either $B \le Z^2$ and $\ell(x) \ge r_* := B^{-\frac{3}{2}}Z^{\frac{1}{3}}$ or $Z^2 \le B \le Z^3$ and $\ell(x) \ge r_* = Z^{-1}$. Introducing partition into two zones $\{x\colon \ell(x) \ge r_*\}$ and $\{x\colon \ell(x) \le 2r_*\}$ adds $\ell^{-2}\phi(x)$ with $\phi(x) = \mathbf{1}_{\{x\colon r_* \le \ell(x) \le 2r_*\}}$, which adds $-CR$ to the right-hand expression of (26.A.12).

Therefore we need to deal with the zone $\{x\colon \ell(x) \le 2r_*\}$. In this zone however we can neglect an external field; indeed, as in Remark 27.4.1 we get the same estimate (27.4.25) but with B intensity of the combined field; however $\int B^2\,dx$ over this zone does not exceed CR. This concludes proof of Statement (i).

Statement (ii) is proven in the same manner as in Appendix 26.A.1. We leave details to the reader. □

28.A.3 Estimates for $(hD_{x_j} - \mu x_j)e(x,y,\tau)|_{x=y}$ for Toy-Model Operator

We will use here notations of Subsection 27.5.1.

Calculations

Let us calculate the required expressions as $X = \mathbb{R}^3$ and $A(x)$ and $V(x)$ are linear. To do this we can consider just Schrödinger operator (acting on vector-functions) and then replace V by $V \pm \mu h$ where μ is the magnetic intensity; since $\sigma_j\sigma_k + \sigma_k\sigma_j = 2\delta_{jk}$ we have to consider scalar a Schrödinger operator. Let us apply calculations of Subsection 16.6.1 with operator

$$H = h^2 D_1^2 + (hD_2 - \mu x_1)^2 + hD_3^2 - 2\alpha x_1 - 2\beta x_3, \tag{28.A.14}$$

where without any loss of the generality we assume that $\alpha \ge 0$, $\beta \ge 0$.

After rescaling $x \mapsto \mu x$, $y \mapsto \mu y$, $t \mapsto \mu t$, $\mu \mapsto 1$ (but we will need to use old μ in calculations), $h \mapsto \hbar = \mu h$ we have $U(x,y,t) = U_{(1)}(x_3, y_3, t) U_{(2)}(x', y', t)$ where from (16.6.4)

$$\begin{gathered} U_{(1)}(x_3, y_3, t) = \\ \frac{1}{2}\mu (2\pi\hbar |t|)^{-\frac{1}{2}} \exp\Bigl(i\hbar^{-1}\bigl(\mu^{-1}\beta t(x_3+y_3) + \frac{1}{8}t^{-1}(x_3-y_3)^2 + \frac{1}{3}\mu^{-2}\beta^2 t^3\bigr)\Bigr); \end{gathered}\tag{28.A.15}$$

and repeating (16.2.9)–(28.A.16) we get

$$U_{(2)}(x,y,t) = i(4\pi\hbar)^{-1}\mu^2 \csc(t)\, e^{i\hbar^{-1}\bar{\phi}_{(2)}(x',y',t)} \tag{28.A.16}$$

with

$$\begin{aligned} \bar{\phi}_{(2)} := &-\frac{1}{4}\cot(t)(x_1-y_1)^2 \\ &+\frac{1}{2}(x_1+y_1+2\alpha\mu^{-1})(x_2-y_2+2t\alpha\mu^{-1}) \\ &-\frac{1}{4}\cot(t)(x_2-y_2+2t\alpha\mu^{-1})^2 - t\alpha^2\mu^{-2}. \end{aligned}\tag{28.A.17}$$

Then

$$U(x,y,t) = i(2\pi h)^{-\frac{3}{2}}|t|^{-\frac{1}{2}}\mu^{\frac{3}{2}} \csc(t)\, e^{i\hbar^{-1}\bar{\phi}(x,y,t)} \tag{28.A.18}$$

with

$$\begin{gathered} \bar{\phi} := -\frac{1}{4}\cot(t)(x_1-y_1)^2 \\ +\frac{1}{2}(x_1+y_1+2\alpha\mu^{-1})(x_2-y_2+2t\alpha\mu^{-1}) - \frac{1}{4}\cot(t)(x_2-y_2+2t\alpha\mu^{-1})^2 - t\alpha^2\mu^{-2} + \\ \mu^{-1}\beta t(x_3+y_3) + \frac{1}{8}t^{-1}(x_3-y_3)^2 + \frac{1}{3}\mu^{-2}\beta^2 t^3\bigr). \end{gathered}\tag{28.A.19}$$

Therefore applying first $\hbar D_{x_1}$, $\hbar D_{x_2}-\mu x_1$, or $\hbar D_{x_3}$ and setting after this $x=y=0$ we conclude that

$$(\hbar D_{x_1}U)|_{x=y=0} = i\alpha\mu^{-1}t\times(2\pi h)^{-\frac{3}{2}}|t|^{-\frac{1}{2}}\mu^{\frac{3}{2}}e^{i\hbar^{-1}\varphi(t)}, \tag{28.A.20$_1$}$$

$$(\hbar D_{x_2}U)|_{x=y=0} = i\alpha\mu^{-1}(1-t\cot(t))\times(2\pi h)^{-\frac{3}{2}}|t|^{-\frac{1}{2}}\mu^{\frac{3}{2}}e^{i\hbar^{-1}\varphi(t)}, \tag{28.A.20$_2$}$$

$$(\hbar D_{x_3}U)|_{x=y=0} = i\beta\mu^{-1}t\times(2\pi h)^{-\frac{3}{2}}|t|^{-\frac{1}{2}}\mu^{\frac{3}{2}}e^{i\hbar^{-1}\varphi(t)} \tag{28.A.20$_3$}$$

with

$$\varphi(t)=\alpha^2\mu^{-2}t-\alpha^2\mu^{-2}t^2\cot(t)+\frac{1}{3}\mu^{-2}\beta^2t^3. \tag{28.A.21}$$

In other words, in comparison with $U|_{x=y=0}$, calculated in Subsection 16.6.1, expressions $(\hbar D_{x_1}U)|_{x=y=0}$, $(\hbar D_{x_2}U)|_{x=y=0}$ and $(\hbar D_{x_3}U)|_{x=y=0}$ acquire factors $\mu^{-1}\alpha t$, $\mu^{-1}\alpha(1-t\cot(t))$ and $\mu^{-1}\beta t$ respectively.

Recall that we had 2 cases: $\mu^2h\le\alpha$ and $\mu^2h\ge\alpha$.

Case $\alpha\ge\mu^2h$

Then for each k, $1\le|k|\le C_0\mu\alpha^{-1}$, the k-th tick contributed no more than

$$C\mu h^{-1}\underbracket{(\mu^2h/\alpha|k|)^{\frac{1}{2}}}\times(\mu/h|k|)^{\frac{1}{2}} \tag{28.A.22}$$

to $F_{t\to\hbar^{-1}\tau}U|_{x=y=0}$ (see Subsection 16.6.2) and then it contributed no more than this multiplied by $|t_k|^{-1}$, i.e.

$$C\mu h^{-1}|k|^{-1}\underbracket{(\mu^2h/\alpha|k|)^{\frac{1}{2}}}\times(\mu/h|k|)^{\frac{1}{2}} \tag{28.A.23}$$

to the corresponding Tauberian expression. Even when we multiply by $\mu^{-1}|k|$, we get (28.A.22) again proportional to $|k|^{-1}$; then summation with respect to k, $1\le|k|\le k^*:=C_0\mu(\alpha+\beta)^{-1}$ [39] returns its value at $k=1$, i.e. $\mu^{\frac{3}{2}}h^{-1}\alpha^{-\frac{1}{2}}$ multiplied by logarithm $(1+|\log k^*|)$ and therefore we arrive to Proposition 28.A.4 below for $j=1,3$.

Let $j=2$. Since $t_k/\cot(t_k)\asymp\alpha^{-1}\mu$ we conclude that contribution of k-th tick does not exceed

$$C\mu h^{-1}|k|^{-1}\underbracket{(\mu^2h/\alpha|k|)^{\frac{1}{2}}}\times(\mu/h|k|)^{\frac{1}{2}} \tag{28.A.24}$$

[39] As $|t|\ge k^*$ we have $\phi'(t)\ge c_1$ and then integrating by parts there we can recover factor $(t/k^*)^{-n}$ thus effectively confining us to integration over $\{t\colon |t|\le k^*\}$. This observation can also improve some results of Sections 16.6–16.10.

and summation by $|k|\ge 1$ returns its value as $|k|=1$ i.e. $C\mu^{\frac{5}{2}}h^{-1}\alpha^{-\frac{1}{2}}$ and therefore we arrive to proposition 28.A.4 below for $j=2$.

Proposition 28.A.4. *Let $\mu h\le \epsilon_0$, $\tau\asymp 1$, $\alpha\ge \mu^2 h$.*
Then

(i) Expression $(hD_{x_2}-\mu x_1)e(x,y,\tau)|_{x=y=0}$ does not exceed $C\mu^{\frac{5}{2}}h^{-1}\alpha^{-\frac{1}{2}}$.

(ii) Expression $hD_{x_j}e(x,y,\tau)|_{x=y=0}$ does not exceed $C\mu^{\frac{3}{2}}h^{-1}\alpha^{\frac{1}{2}}(1+|\log \mu(\alpha+\beta)^{-1}|)$, and $C\mu^{\frac{3}{2}}h^{-1}\beta\alpha^{-\frac{1}{2}}(1+|\log \mu(\alpha+\beta)^{-1}|)$ for $j=1,3$ respectively.

Case $\alpha\le \mu^2 h$

If $\mu^2 h\ge \alpha$, then the same arguments work only for $\bar{k}:=\mu^2 h\alpha^{-1}\le |k|\le k^*$, resulting in contributions $C\mu^{\frac{3}{2}}h^{-1}\alpha^{\frac{1}{2}}(1+|\log k^*\bar{k}^{-1}|)$, $C\mu^{\frac{1}{2}}h^{-2}\alpha^{\frac{1}{2}}$, and $C\mu^{\frac{3}{2}}h^{-1}\beta\alpha^{-\frac{1}{2}}(1+|\log k^*\bar{k}^{-1}|)$ for $j=1,2,3$ respectively if $\bar{k}\le k^*$ (i.e. $\mu h\beta\le\alpha$) or 0 otherwise.

Let $1\le |k|\le \bar{k}$. We mainly consider the most difficult case $j=2$ and (as $|t|\ge\epsilon_0$) only term arising from $-\alpha\mu^{-1}t\cot(t)$ factor, namely

$$\alpha\mu^{-1}\times \mu^{\frac{3}{2}}h^{-\frac{3}{2}}\int |t|^{-\frac{1}{2}}\cos(t)(\sin(t))^{-2}e^{i\hbar^{-1}(\varphi(t)-t\tau)}\,dt, \tag{28.A.25}$$

where we took into account that we need to divide by t and skipped a constant factor.

Consider first (28.A.25) with integration over interval $\{t\colon |t-t_k|\le s_k\}$ near t_k. Observe that

$$\phi'(t)=(\sin(t))^{-2}\alpha^2\mu^{-2}t^2-2t(\sin(t))^{-1}\alpha^2\mu^{-2}t^2+\beta^2t^2 \tag{28.A.26}$$

and transform (28.A.25) into

$$\alpha^{-1}\mu^{\frac{7}{2}}h^{-\frac{1}{2}}\int_{t_k-s_k}^{t_k+s_k}|t|^{-\frac{5}{2}}\cos(t)\partial_t\bigl[e^{i\hbar^{-1}(\varphi(t)-t\tau)}\bigr]\,dt \tag{28.A.27}$$
$$+\alpha^{-1}\mu^{\frac{5}{2}}h^{-\frac{3}{2}}\int_{t_k-s_k}^{t_k+s_k}|t|^{-\frac{5}{2}}\cos(t)\bigl[2t(\sin(t))^{-1}\alpha^2\mu^{-2}-\beta^2t^2+\tau\bigr]e^{i\hbar^{-1}(\varphi(t)-t\tau)}.$$

Integrating the first term by parts we get a non-integral term

$$\alpha^{-1}\mu^{\frac{7}{2}}h^{-\frac{1}{2}}|t|^{-\frac{5}{2}}\cos(t)e^{i\hbar^{-1}(\varphi(t)-t\tau)}\Bigr|_{t=t_k-s_k}^{t=t_k+s_k} \tag{28.A.28}$$

and we get an integral term

$$\begin{aligned}\alpha^{-1}\mu^{\frac{5}{2}}h^{-\frac{3}{2}}\int_{t_k-s_k}^{t_k+s_k}\Bigl[\mu h\partial_t\bigl[|t|^{-\frac{5}{2}}\cos(t)\bigr]\\ +|t|^{-\frac{5}{2}}\cos(t)\bigl[2t(\sin(t))^{-1}\alpha^2\mu^{-2}-\beta^2t^2+\tau\bigr]\Bigr]e^{i\hbar^{-1}(\varphi(t)-t\tau)}\,dt\\ =2\alpha\mu^{\frac{1}{2}}h^{-\frac{3}{2}}\int_{t_k-s_k}^{t_k+s_k}|t|^{-\frac{3}{2}}\cot(t)e^{i\hbar^{-1}(\varphi(t)-t\tau)}\,dt+O\bigl(\alpha^{-1}\mu^{\frac{5}{2}}h^{-\frac{3}{2}}s_k|k|^{-\frac{5}{2}}\bigr).\end{aligned}\tag{28.A.29}$$

Repeating the same trick we can eliminate the first term in the right-most expression. Therefore we arrive to (28.A.28) with $O\bigl(\alpha^{-1}\mu^{\frac{5}{2}}h^{-\frac{3}{2}}s_k|k|^{-\frac{5}{2}}\bigr)$ error. When $s_k\asymp\alpha^2\mu^{-3}h^{-1}k^2$ we get

$$C\mu^{\frac{3}{2}}h^{-\frac{3}{2}}\times(\alpha/\mu^2h)|k|^{-\frac{1}{2}}\tag{28.A.30}$$

error.

On the other hand, consider integral over $[t_k+s_k,t_{k+1}-s_{k+1}]$, $k\ne 0$. Decomposing $e^{i\mu^{-1}h^{-1}(\phi(t)-t\tau)}$ into Taylor series with respect to $\alpha^2h^{-1}\mu^{-3}\cot(t)$ one can prove easily that expression in question is

$$\alpha^{-1}\mu^{\frac{7}{2}}h^{-\frac{1}{2}}|t|^{-\frac{5}{2}}\cos(t)\bigl(e^{i\hbar^{-1}(\varphi(t)-t\tau)}-e^{i\hbar^{-1}(\varphi_{(1)}(t)-t\tau)}\bigr)\Bigr|_{t=t_k+s_k}^{t=t_{k+1}-s_{k+1}}$$

with $\varphi_{(1)}(t)=\frac{1}{3}\mu^{-2}\beta^2t^3$ and with error not exceeding (28.A.30) multiplied by $(1+|\log s_k|)$:

$$C\mu^{\frac{3}{2}}h^{-\frac{3}{2}}\times(\alpha/\mu^2h)|k|^{-\frac{1}{2}}\times(1+|\log(\alpha^2\mu^{-3}h^{-1}k^2)|).\tag{28.A.31}$$

So non-integral terms with φ cancel one another because by the similar arguments we can also cover $[0,t_1-s_1]$ and $[t_{-1}+s_{-1}]$ and due to non-singularity of $t^{-1}(1-t\cot(t))\csc(t)$ at $t=0$ there will be no non-integral terms with $k=0$. So we are left with

$$-\alpha^{-1}\mu^{\frac{7}{2}}h^{-\frac{1}{2}}|t|^{-\frac{5}{2}}\cos(t)e^{i\hbar^{-1}(\varphi_{(1)}(t)-t\tau)})\Bigr|_{t=t_k-s_k}^{t=t_k+s_k}$$

and their absolute values do not exceed (28.A.30).

Finally, summation of (28.A.31) by $k:1\le|k|\le\min(\bar{k},k^*)$ returns

$$\begin{aligned}C\mu^{\frac{3}{2}}h^{-\frac{3}{2}}(\alpha/\mu^2h)^{\frac{1}{2}}\\ \times\begin{cases}(1+|\log(\mu h)|) & \beta\mu h\le\alpha,\\ (\alpha/\beta\mu h)^{\frac{1}{2}}(1+|\log(\mu h)|+|\log(\alpha/\beta\mu h)|) & \beta\mu h\ge\alpha.\end{cases}\end{aligned}\tag{28.A.32}$$

and we arrive to Proposition 28.A.5 below for $j=2$:

Proposition 28.A.5. *Let* $\mu h \le \epsilon_0$, $\tau \asymp 1$, *and* $\alpha \le \mu^2 h$.
Then

(i) Expression $(hD_{x_2} - \mu x_1) e(x,y,\tau)|_{x=y=0}$ *does not exceed* (28.A.32).

(ii) Expression $hD_{x_3} e(x,y,\tau)|_{x=y=0}$ *does not exceed*

$$C\left\{\begin{aligned} &\mu^{\frac{3}{2}} h^{-1}\beta\alpha^{-\frac{1}{2}}(1+|\log(\alpha/\beta\mu h)|) &&\textit{if}\ \ \beta\mu h\le\alpha,\\ &\mu h^{-\frac{3}{2}}\beta^{\frac{1}{2}} &&\textit{if}\ \ \beta\mu h\ge\alpha.\end{aligned}\right. \tag{28.A.33}$$

(iii) Expression $hD_{x_1} e(x,y,\tau)|_{x=y=0}$ *does not exceed*

$$C\left\{\begin{aligned} &\mu^{\frac{3}{2}} h^{-1}\alpha^{\frac{1}{2}}(1+|\log(\alpha/\beta\mu h)|) &&\textit{if}\ \ \beta\mu h\le\alpha,\\ &\mu h^{-\frac{3}{2}}\alpha^{\frac{1}{2}} &&\textit{if}\ \ \beta\mu h\ge\alpha.\end{aligned}\right. \tag{28.A.34}$$

Case $\mu h \ge \epsilon_0$

If $\mu h \ge \epsilon_0$ we consider a different representation: namely (16.2.15) for a spectral projector in dimension 2 (again after rescaling where we scale e_* as functions rather than Schwartz kernels):

$$\begin{multlined} e_{(2)}(x',y',\tau) = \\ (2\pi)^{-1}\mu h^{-1}\sum_{m\in\mathbb{Z}^+}\int \upsilon_m\bigl(\eta+\mu^{-\frac{1}{2}}h^{-\frac{1}{2}}(x_1-y_1)\bigr)\upsilon_m\bigl(\eta-\mu^{-\frac{1}{2}}h^{-\frac{1}{2}}(x_1-y_1)\bigr)\\ \times\theta\Bigl(\tau-\alpha\mu^{-1}(x_1+y_1)-2\alpha\mu^{-\frac{1}{2}}h^{\frac{1}{2}}\eta-\alpha^2\mu^{-2}-2m\mu h\Bigr)e^{i\mu^{-\frac{1}{2}}h^{-\frac{1}{2}}(x_2-y_2)\eta}\,d\eta,\end{multlined} \tag{28.A.35}$$

where we also replaced $H_{(2)}$ by $H_{(2)}-\mu h$ and τ by $\mu h+\tau$. Since

$$e(x,y,\tau) = e_{(2)}(x',y',.)*_\tau e_{(1)}(x_3,y_3,.), \tag{28.A.36}$$

where $e_{(1)}(x_3,y_3,\tau)$ is a Schwartz kernel of the spectral projector of 1-dimensional operator

$$\mu^2 h^2 D_3^2 - 2\beta\mu^{-1}x_3, \tag{28.A.37}$$

we conclude that

$$\begin{multlined} e(x,y,\tau) \\ = (2\pi)^{-1}\mu h^{-1}\sum_{m\in\mathbb{Z}^+}\int \upsilon_m\bigl(\eta+\mu^{-\frac{1}{2}}h^{-\frac{1}{2}}(x_1-y_1)\bigr)\upsilon_m\bigl(\eta-\mu^{-\frac{1}{2}}h^{-\frac{1}{2}}(x_1-y_1)\bigr)\\ \times e_{(1)}\Bigl(x_3,y_3,\tau-\alpha\mu^{-1}(x_1+y_1)-2\alpha\mu^{-\frac{1}{2}}h^{\frac{1}{2}}\eta-\alpha^2\mu^{-2}-2m\mu h\Bigr)e^{i\mu^{-\frac{1}{2}}h^{-\frac{1}{2}}(x_2-y_2)\eta}\,d\eta.\end{multlined} \tag{28.A.38}$$

Then

$$(\mu h D_{x_2} - x_1) e(x,y,\tau)\bigr|_{x=y=0} \tag{28.A.39}$$
$$= (2\pi)^{-1}\mu^{\frac{3}{2}} h^{-\frac{1}{2}} \sum_{m\in\mathbb{Z}^+} \int \upsilon_m^2(\eta)\eta\times e_{(1)}\Bigl(0,0,\tau-2\alpha\mu^{-\frac{1}{2}}h^{\frac{1}{2}}\eta-\alpha^2\mu^{-2}-2m\mu h\Bigr)\,d\eta$$

and since $\upsilon_m(.)$ is an even (odd) function for even (odd) m we can replace $e_{(1)}(0,0,\tau' - 2\alpha\mu^{-\frac{1}{2}}h^{\frac{1}{2}}\eta)$ by

$$e_{(1)}(0,0,\tau' - 2\alpha\mu^{-\frac{1}{2}}h^{\frac{1}{2}}\eta) - e_{(1)}(0,0,\tau' + 2\alpha\mu^{-\frac{1}{2}}h^{\frac{1}{2}}\eta). \tag{28.A.40}$$

In virtue of Subsubsection 5.2.1.3 *Asymptotics without Spatial Mollification* we know that an absolute value of this expression does not exceed $Ch^{-\frac{1}{2}}\alpha^{\frac{1}{2}}$ [40] we arrive to estimate[41]

$$|(hD_{x_2} - \mu x_1) e(x,y,\tau)\bigr|_{x=y=0}| \le C\mu^{\frac{3}{2}} h^{-1}\alpha^{\frac{1}{2}}. \tag{28.A.41}$$

Further,

$$\mu h D_{x_1} e(x,y,\tau)\bigr|_{x=y=0} \tag{28.A.42}$$
$$= i(2\pi)^{-1}\alpha\mu \sum_{m\in\mathbb{Z}^+} \int \upsilon_m^2(\eta)\times \partial_\tau e_{(1)}\bigl(0,0,\tau-2\alpha\mu^{-\frac{1}{2}}h^{\frac{1}{2}}\eta-\alpha^2\mu^{-2}-2m\mu h\bigr)\,d\eta$$
$$= i(2\pi)^{-1}\mu^{\frac{3}{2}} h^{-\frac{1}{2}} \sum_{m\in\mathbb{Z}^+} \int \upsilon_m(\eta)\upsilon_m'(\eta)\times e_{(1)}\bigl(0,0,\tau-2\alpha\mu^{-\frac{1}{2}}h^{\frac{1}{2}}\eta-\alpha^2\mu^{-2}-2m\mu h\bigr)\,d\eta$$

and using the same arguments we arrive to estimate[41]

$$|hD_{x_1} e(x,y,\tau)\bigr|_{x=y=0}| \le C\mu^{\frac{3}{2}} h^{-1}\alpha^{\frac{1}{2}}. \tag{28.A.43}$$

Finally,

$$\mu h D_{x_3} e(x,y,\tau)\bigr|_{x=y=0} = (2\pi)^{-1}\mu h^{-1} \sum_{m\in\mathbb{Z}^+} \int \upsilon_m^2(\eta) \tag{28.A.44}$$
$$\times\, \underbrace{\mu h D_{x_3} e_{(1)}\bigl(x_3,y_3,\tau-2\alpha\mu^{-\frac{1}{2}}h^{\frac{1}{2}}\eta-\alpha^2\mu^{-2}-2m\mu h\bigr)\bigr|_{x_3=y_3=0}}\,d\eta$$

[40] Only in the worst case when $|\tau - 2m\mu h|$ is not disjoint from 0.
[41] In the non-rescaled coordinates.

and again in virtue of Subsubsection 5.2.1.3 *Asymptotics without Spatial Mollification* we know that an absolute value of selected expression does not exceed $Ch^{-\frac{1}{2}}\beta^{\frac{1}{2}}$ [42] and we arrive to estimate[41]

$$|hD_{x_3}e(x,y,\tau)\bigr|_{x=y=0}| \le C\mu h^{-\frac{3}{2}}\beta^{\frac{1}{2}}. \tag{28.A.45}$$

Therefore we have proven

Proposition 28.A.6. *Let* $\mu h\ge 1$, $\alpha\le 1$, $\beta\le 1$, $|\tau|\le c_0$. *Then for operator* $(H-\mu h)$ *estimates* (28.A.41), (28.A.43) *and* (28.A.45) *hold.*

Tauberian Estimates

Remark 28.A.7. Assume now that all assumptions are fulfilled only in $B(0,\ell)$ rather than in $\mathbb{R}^3$. Then there is also a Tauberian estimate which should be added to Weyl estimate. This Tauberian estimate (the same for all $j=1,2,3$) coincides with the Tauberian estimate was calculated in Chapter 16. Namely

(i) For $\mu h\le 1$, $\ell\ge C_0\mu^{-1}$ this Tauberian estimate was calculated in Proposition 16.6.2(ii)[41].

(ii) For $\mu h\ge 1$, $\ell\ge C_0 h$ this Tauberian estimate was calculated in Proposition 16.6.7(i) and corollary 16.6.8(i)[41] and it does not exceed $C\mu h^{-\frac{3}{2}}\ell^{-1}$.

[42] Without applying $(hD_j-\mu A_j(x))$ but it does not matter.

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Part XII

Articles

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Spectral Asymptotics for the Semiclassical Dirichlet to Neumann Operator *,†

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Abstract

Let M be a compact Riemannian manifold with smooth boundary, and let $R(\lambda)$ be the Dirichlet-to-Neumann operator at frequency λ. The semiclassical Dirichlet-to-Neumann operator $R_{\mathsf{scl}}(\lambda)$ is defined to be $\lambda^{-1}R(\lambda)$. We obtain a leading asymptotic for the spectral counting function for $R_{\mathsf{scl}}(\lambda)$ in an interval $[a_1, a_2)$ as $\lambda \to \infty$, under the assumption that the measure of periodic billiards on T^*M is zero. The asymptotic takes the form

$$\mathsf{N}(\lambda; a_1, a_2) = \bigl(\kappa(a_2) - \kappa(a_1)\bigr)\,\mathsf{vol}'(\partial M)\lambda^{d-1} + o(\lambda^{d-1}),$$

where $\kappa(a)$ is given explicitly by

$$\kappa(a) = \frac{\omega_{d-1}}{(2\pi)^{d-1}}\biggl(-\frac{1}{2\pi}\int_{-1}^{1} (1-\eta^2)^{(d-1)/2}\frac{a}{a^2+\eta^2}\,d\eta \\ - \frac{1}{4} + H(a)(1+a^2)^{(d-1)/2}\biggr).$$

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1 Introduction

Let M be a Riemannian manifold with boundary. The Dirichlet-to-Neumann operator is a family of operators defined on $L^2(\partial M)$ depending on the parameter $\lambda \geq 0$. It is defined as follows: given $f \in L^2(\partial M)$, we solve the equation (if possible)

$$(\Delta - \lambda^2)u = 0 \quad \text{on} \quad M, \qquad u|_{\partial M} = f. \tag{1.1}$$

Then the Dirichlet-to-Neumann operator at frequency λ is the map

$$R(\lambda) : f \mapsto -\partial_\nu u|_{\partial M}. \tag{1.2}$$

Here ∂_ν is the interior unit normal derivative, and Δ is the positive Laplacian on M.

It is well known that $R(\lambda)$ is a self-adjoint, semi-bounded from below pseudodifferential operator of order 1 on $L^2(\partial M)$, with domain $H^1(\partial M)$. It therefore has discrete spectrum accumulating only at $+\infty$. The Dirichlet-to-Neumann operator and closely related operators are important in a number of areas of mathematical analysis including inverse problems (such as Calderón's problem [Cal]), domain decomposition problems (such as the determinant gluing formula of Burghelea-Friedlander-Kappeler [BFK]), and spectral asymptotics (see e.g. [Fried]).

In this paper, we are interested in the spectral asymptotics of $R(\lambda)$ in the high-frequency limit, $\lambda \to \infty$. Let us recall standard spectral asymptotics for elliptic differential operators, for simplicity in the simplest case of a positive self-adjoint second order scalar operator. Suppose that Q is such an operator on a manifold M of dimension d, with principal symbol q. Then in the case that M is closed, we have an asymptotic for the number $\mathsf{N}(\lambda)$ of eigenvalues of Q (counted with multiplicity) less than λ^2:

$$\begin{aligned} \mathsf{N}(\lambda) &= (2\pi)^{-d} \operatorname{vol}\{(x,\xi) \in T^*M \mid q(x,\xi) \leq \lambda^2\} + O(\lambda^{d-1}) \\ &= \Big(\frac{\lambda}{2\pi}\Big)^d \operatorname{vol}\{(x,\xi) \in T^*M \mid q(x,\xi) \leq 1\} + O(\lambda^{d-1}), \end{aligned} \tag{1.3}$$

where the equality of the two expressions on the RHS is a simple consequence of the homogeneity of q. Moreover, if the set of periodic geodesics has measure zero, then there is a two-term expansion of the form

$$\Big(\frac{\lambda}{2\pi}\Big)^d \operatorname{vol}\{(x,\xi) \in T^*M \mid q(x,\xi) \leq 1\} + \frac{\lambda^{d-1}}{(2\pi)^d} \int_{\{q=1\}} \operatorname{sub}(Q) + o(\lambda^{d-1})$$

where $\mathsf{sub}(Q)$ is the subprincipal symbol of Q [DuGu]. This was generalised to the case of manifolds with boundary by the second author [Ivr1]. For simplicity we state the result in the case that $Q = \Delta$ is the (positive) metric Laplacian, which satisfies $\mathsf{sub}(\Delta) = 0$. Then Δ is a self-adjoint operator under either Dirichlet $(-)$ or Neumann $(+)$ boundary conditions, and if the set of periodic generalised bicharacteristics has measure zero, we get a two-term expansion for $\mathsf{N}_\Delta(\lambda)$ of the form

$$(\frac{\lambda}{2\pi})^d \operatorname{vol} B^*M \pm \frac{1}{4}(\frac{\lambda}{2\pi})^{d-1} \operatorname{vol} B^*\partial M + o(\lambda^{d-1}). \tag{1.4}$$

These statements can be generalized to the semiclassical setting. Consider a classical Schrödinger operator on M, $P = h^2\Delta + V(x) - 1$, where $h > 0$ is a small parameter ("Planck's constant") and V is a smooth real-valued function. We consider the asymptotic behaviour $\mathsf{N}_h^-(P)$ of the number of negative eigenvalues of P as $h \to 0$. This is equivalent to the problem above if $h = \lambda^{-1}$ and V is identically zero. Define $p(x,\xi)$ to be the semiclassical symbol of P, i.e. $p = |\xi|^2_{g(x)} + V(x) - 1$. Then, if M is closed, under the assumption that the measure of periodic bicharacteristics of P is zero in T^*M, and that 0 is a regular value for p, we have

$$\mathsf{N}_h^-(P) = (2\pi h)^{-d} \operatorname{vol}\{(x,\xi) \in T^*M \mid p(x,\xi) \le 0\} + O(h^{1-d}). \tag{1.5}$$

Moreover, for manifolds with boundary, we have an analogue of (1.4): under either Dirichlet $(-)$ or Neumann $(+)$ boundary conditions, if the set of periodic generalised bicharacteristics has measure zero, we get a two-term expansion for $\mathsf{N}_h^-(P)$ (where here we understand the self-adjoint realization of P with either Dirichlet or Neumann boundary condition) of the form

$$(2\pi h)^{-d} \operatorname{vol}\{(x,\xi) \in T^*M \mid p(x,\xi) \le 0\} \pm \frac{1}{4}(2\pi h)^{1-d} \operatorname{vol} \mathcal{H} + o(h^{1-d}), \tag{1.6}$$

where $\mathcal{H} \subset T^*(\partial M)$ is the hyperbolic region in the boundary, that is, the projection of the set $\{(x,\xi) \mid p(x,\xi) \le 0\} \cap T^*_{\partial M}M$ to $T^*\partial M$.

From the semiclassical point of view, since $R(\lambda)$ is a first order operator, it makes sense to consider $R_{\mathsf{scl}}(\lambda) := \lambda^{-1}R(\lambda)$ (for $\lambda > 0$), which we call the semiclassical Dirichlet-to-Neumann operator. Like $R(\lambda)$, it is a self-adjoint, semi-bounded from below operator on $L^2(\partial M)$, with discrete spectrum accumulating only at $+\infty$. The goal of this paper is to investigate the spectral asymptotics of $R_{\mathsf{scl}}(\lambda)$, that is, the asymptotics of

$$\mathsf{N}(\lambda; a_1, a_2) := \#\{\beta :\ \beta \text{ is an eigenvalue of } \ R_{\mathsf{scl}}(\lambda),\ a_1 \le \beta < a_2\}, \tag{1.7}$$

the number of eigenvalues of $R_{\mathrm{scl}}(\lambda)$ in the interval $[a_1, a_2)$, as $\lambda \to \infty$.

Both $R(\lambda)$ and $R_{\mathrm{scl}}(\lambda)$ have the disadvantage that they are undefined whenever λ^2 is a Dirichlet eigenvalue, since then (1.1) is not solvable for arbitrary $f \in H^1(M)$. Indeed, when λ^2 is a Dirichlet eigenvalue, a necessary condition for solvability of (1.1) is that f is orthogonal to the normal derivatives of Dirichlet eigenfunctions at frequency λ. To overcome this issue, we introduce the *Cayley transform* of $R_{\mathrm{scl}}(\lambda)$: we define

$$C(\lambda) = (R_{\mathrm{scl}}(\lambda) - i)(R_{\mathrm{scl}}(\lambda) + i)^{-1}. \tag{1.8}$$

This family of operators is related to impedance boundary conditions: we have $C(\lambda)f = g$ if and only if there is a function u on M satisfying

$$(\Delta - \lambda^2)u = 0 \tag{1.9}$$

and

$$\frac{1}{2}(\lambda^{-1}\partial_\nu u - iu) = f, \qquad \frac{1}{2}(\lambda^{-1}\partial_\nu u + iu) = g. \tag{1.10$_{1,2}$}$$

As observed in [BH], $C(\lambda)$ is a well-defined analytic family of operators for λ in a neighbourhood of the positive real axis, which is unitary on the real axis. In particular, it is well-defined even when λ^2 is a Dirichlet eigenvalue of the Laplacian on M. As a unitary operator, $C(\lambda)$, $\lambda > 0$, has its spectrum on the unit circle, and as $R_{\mathrm{scl}}(\lambda)$ has discrete spectrum accumulating only at ∞, it follows that the spectrum of $C(\lambda)$ is discrete on the unit circle except at the point 1. Our question can be formulated in terms of $C(\lambda)$: given two angles θ_1, θ_2 satisfying $0 < \theta_1 < \theta_2 < 2\pi$, what is the leading asymptotic for

$$\tilde{\mathsf{N}}(\lambda; \theta_1, \theta_2) := \#\{e^{i\theta} : e^{i\theta} \text{ is an eigenvalue of } C(\lambda),\ \theta_1 \le \theta < \theta_2\} \tag{1.11}$$

the number of eigenvalues of $C(\lambda)$ in the interval $\{e^{i\theta} : \theta \in [\theta_1, \theta_2)\}$ of the unit circle, as $\lambda \to \infty$. Clearly, we have

$$\tilde{\mathsf{N}}(\lambda; \theta_1, \theta_2) = \mathsf{N}(\lambda; a_1, a_2), \text{ where } e^{i\theta_j} = \frac{a_j - i}{a_j + i}, \text{ i.e. } a_j = -\cot\left(\frac{\theta_j}{2}\right). \tag{1.12}$$

To answer this question we relate it to a standard semiclassical eigenvalue counting problem on M. To state the next result, we first define the self-adjoint operator $P_{a,h}$ on $L^2(M)$ by

$$\mathfrak{D}(P_{a,h}) = \{u \in H^2(M) : (h\partial_\nu + a)u = 0 \text{ at } \partial M\}, \tag{1.13}$$

$$P_{a,h}(u) = (h^2\Delta - 1)u, \quad u \in \mathfrak{D}(P_{a,h}). \tag{1.14}$$

It is the self-adjoint operator associated to the semi-bounded quadratic form

$$h^2\|\nabla u\|_M^2 - \|u\|_M^2 - ha\|u\|_{\partial M}^2. \tag{1.15}$$

The operator $P_{a,h}$ is linked with the semiclassical Dirichlet-to-Neumann operator as follows: if f is an eigenfunction of $R_{\mathrm{scl}}(\lambda)$ with eigenvalue a, then the corresponding Helmholtz function u defined by (1.1) is in the domain (1.13) of $P_{a,h}$, and $P_{a,h}u = 0$ (where $h = \lambda^{-1}$).

Then we have the following result, proved in Section 2.

Proposition 1.1. *Let $h = \lambda^{-1}$. Assume $0 < \theta_1 < \theta_2 < 2\pi$. Then the number of eigenvalues of $C(\lambda)$ in the interval $J_{\theta_1,\theta_2} := \{e^{i\theta} : \theta \in [\theta_1, \theta_2)\}$ is equal to*

$$\tilde{\mathsf{N}}(\lambda; \theta_1, \theta_2) = \mathsf{N}(\lambda; a_1, a_2) = \mathsf{N}_h^-(a_2) - \mathsf{N}_h^-(a_1), \tag{1.16}$$

where $a_j = -\cot(\theta_j/2)$ and

$$\mathsf{N}_h^-(a) := \#\{\mu : \mu \text{ is an eigenvalue of } P_{a,h},\ \mu < 0\}. \tag{1.17}$$

Having thus reduced the problem to a standard question about semiclassical spectral asymptotics, we obtain (after some calculations in Section 3) our main result.

Theorem 1.2. *(i) The following estimate for the quantity (1.11) holds:*

$$\mathsf{N}(\lambda; a_1, a_2) = O(\lambda^{d-1}); \tag{1.18}$$

(ii) Further, if the set of periodic billiards on M has measure 0 then the following asymptotic holds as $\lambda \to +\infty$:

$$\mathsf{N}(\lambda; a_1, a_2) = \big(\kappa(a_2) - \kappa(a_1)\big)\,\mathrm{vol}'(\partial M)\lambda^{d-1} + o(\lambda^{d-1}), \tag{1.19}$$

where $\kappa(a)$ is given explicitly by

$$\kappa(a) = \frac{\omega_{d-1}}{(2\pi)^{d-1}}\left(-\frac{1}{2\pi}\int_{-1}^{1} (1-\eta^2)^{(d-1)/2}\frac{a}{a^2+\eta^2}\,d\eta - \frac{1}{4} + H(a)(1+a^2)^{(d-1)/2}\right). \tag{1.20}$$

Here $H(\cdot)$ is the Heaviside function, ω_d is the volume of the unit ball in $\mathbb{R}^d$, and $\mathrm{vol}(M)$ and $\mathrm{vol}'(\partial M)$ are d-dimensional volume of M and $(d-1)$-dimensional volume of ∂M respectively.

(iii) In the case $d = 3$, we can evaluate this integral exactly and we find that

$$\kappa(a) = \frac{1}{4\pi}\Big(-\frac{1}{4} - \frac{1}{\pi}\operatorname{arccot}(a)(1 + a^2) + (1 + a^2) + \frac{1}{\pi}a\Big) \tag{1.21}$$

where arccot *has range* $(0, \pi)$*. This is simpler expressed in terms of* θ*. Defining* $\tilde{\kappa}(\theta) = \kappa(a)$ *where* $a = -\cot(\theta/2) = \cot(\pi - \theta/2)$*, we have (still under the zero-measure assumption on periodic billiards)*

$$\tilde{\mathsf{N}}(\lambda; \theta_1, \theta_2) = \big(\tilde{\kappa}(\theta_2) - \tilde{\kappa}(\theta_1)\big)\operatorname{vol}'(\partial M)\lambda^2 + o(\lambda^2), \tag{1.22}$$

$$\tilde{\kappa}(\theta) = \frac{1}{4\pi}\Big(- \frac{1}{4} + \frac{1}{2\pi}\big(\frac{\theta - \sin\theta}{\sin^2(\theta/2)}\big)\Big). \tag{1.23}$$

Remark 1.3. It looks disheartening that we only get an upper bound in case (i) and only a "o" remainder under a global geometric condition, but it is the nature of the beast.

In regards to case (i), consider M a hemisphere; then for $\lambda_n^2 = n(n+d-1)$ with $n \in \mathbb{Z}^+$ the operator $R(\lambda)$ has eigenvalue 0 of multiplicity $\asymp n^{d-1}$, hence $N(\lambda; a_1, a_2)$ jumps by at least $c\lambda^{d-1}$ as a_1 or a_2 crosses zero. Therefore, in this case, we do not have an asymptotic, but only an estimate.

In regards to case (ii), we believe that the "o" remainder is the best that can be achieved using current technology. To justify this, consider the problem of finding the spectral asymptotics of the semiclassical Dirichlet-to-Neumann operator for the operator $\Delta + \lambda^2$, instead of $\Delta - \lambda^2$ (for real λ). In this case, one can readily check that the semiclassical Dirichlet-to-Neumann operator is a semiclassically elliptic pseudodifferential operator on the boundary, with principal symbol $\sqrt{1 + h^2\Delta_{\partial M}}$. Then standard spectral asymptotics hold for this operator, and we would get a remainder term $O(\lambda^{d-2})$. However, for the operator $\Delta - \lambda^2$, the semiclassical Dirichlet-to-Neumann operator is only microlocally elliptic in the region $\{(y, \eta) \mid |\eta|_{g'} > 1\} \subset T^*\partial M$, where g' is the induced metric on the boundary. It is hyperbolic in the region where $|\eta|_{g'} < 1$, and that means there is (currently) no machinery for *directly* tackling its spectral asymptotics. Instead, we proceed by relating it to the spectral asymptotics for the interior problem with a family of boundary conditions depending on the spectral parameter a. This means that the problem is in some sense really d-dimensional, and our $o(\lambda^{d-1})$ remainder is the "ghost" of d-dimensional spectral asymptotics, in which the principal, Weyl term cancels under taking the difference (1.16), and all we are left with is the second term — and only under the global geometric assumption of measure zero periodic billiard trajectories.

We note that under stronger assumptions on the billiard flow, the remainder could be improved, for example to $O(\lambda^{d-1-\delta})$ for some $\delta > 0$ in the case of a Euclidean ellipse or elliptical annulus — see Section 7.4 of [Ivr4].

Remark 1.4. One can consider eigenvalues of operator $\rho\lambda^{-1}R(\lambda)$ with $\rho > 0$ smooth on ∂M; then estimates (3.1), (1.18) and asymptotics (3.2), (1.19) hold in the frameworks of Statement (i) and (ii) of Theorem 1.2 respectively albeit with $\kappa(a)\operatorname{vol}'(\partial M)$ replaced by

$$\int_{\partial M} \kappa(\rho(x')a)\, d\sigma$$

where $d\sigma$ is a natural measure on ∂M; however without this condition $\rho > 0$ problem may be much more challenging; even self-adjointness is by no means guaranteed.

Remark 1.5. Operators of the form $P_{a,h}$ were considered by Frank and Geisinger [FG]. They showed that the trace of the negative part of $P_{a,h}$ has a two-term expansion as $h \to 0$ regardless of dynamical assumptions[1)], and the second term in their expansion (the $L_d^{(2)}$ term of [FG, Theorem 1.1]) is closely related to $\kappa(a)$ — see Remark 3.4.

Remark 1.6. We can rephrase Theorem 1.2 in terms of a limiting measure on the unit circle. For each $\lambda > 0$, let $\mu(h)$, $h = \lambda^{-1}$, denote the atomic measure determined by the spectrum of $C(\lambda)$:

$$\mu(h) = (2\pi h)^{d-1} \sum_{e^{i\theta_j}\in \operatorname{spec} C(h^{-1})} \delta(\theta - \theta_j), \tag{1.24}$$

where we include each eigenvalue according to its multiplicity as usual. Then Theorem 1.2 can be expressed in the following way: the measures $\mu(h)$ converge in the weak-$*$ topology as $h \to 0$ to the measure

$$\omega_{d-1}\operatorname{vol}'(\partial M)\frac{d}{d\theta}\tilde{\kappa}(\theta)d\theta \quad \text{on } (0, 2\pi), \text{ that is on } S^1 \setminus \{1\}. \tag{1.25}$$

1) The fact that Frank and Geisinger obtain a second term regardless of dynamical assumptions is simply due to the fact that they study $\operatorname{Tr} f(P_{a,h})$ with $f(\lambda) = -\lambda H(-\lambda)$ (H is the Heaviside function), which is one order smoother than $f(\lambda) = H(-\lambda)$.

In particular, this measure is absolutely continuous, and finite away from $e^{i\theta} = 1$ with an infinite accumulation of mass as $\theta \uparrow 2\pi$. In this form, we can compare our result with results on the semiclassical spectral asymptotics of scattering matrices. In [DGHH] and [GHZ], the scattering matrix $S_h(E)$ at energy E for the Schrödinger operator $h^2\Delta + V(x)$ on $\mathbb{R}^d$ was studied in the semiclassical limit $h \to 0$. Assuming that V is smooth and compactly supported, that E is a nontrapping energy level, and that the set of periodic trajectories of the classical scattering transformation on T^*S^{d-1} has measure zero, it was shown that the measure $\mu(h)$ defined by (1.24) converged weak-$*$ to a uniform measure on $S^1 \setminus \{1\}$, with an atom of infinite mass at the point 1. On the other hand, for polynomially decaying potentials, it was shown by Sobolev and Yafaev [H-SoYa] in the case of central potentials and by Gell-Redman and the first author more generally [GRH] that there is a limiting measure which is nonuniform, and is qualitatively similar to the measure for $C(h^{-1})$ above in that it is finite away from 1, with an infinite accumulation of mass at 1 from one side.

2 Reduction to Semiclassical Spectral Asymptotics

In this section we prove Proposition 1.1. This result actually follows directly from the Birman-Schwinger principle. As some readers may not be familiar with this, we give the details.

Proof of Proposition 1.1. We begin by recalling that the operator $P_{a,h}$ is the self-adjoint operator associated to the quadratic form (1.15), that is,

$$Q_{a,h}(u) := h^2\|\nabla u\|_M^2 - \|u\|_M^2 - ha\|u\|_{\partial M}^2.$$

We recall the min-max characterization of eigenvalues: the nth eigenvalue $\mu_n(a, h)$ of $P_{a,h}$ is equal to the infimum of

$$\sup_{v \in V, \|v\|=1} Q_{a,h}(v)$$

over all subspaces $V \in H^1(M)$ of dimension n. The monotonicity of $Q_{a,h}$ in a, for fixed h, shows that the eigenvalues are monotone nonincreasing with a. In fact, they are strictly decreasing, which follows from the fact

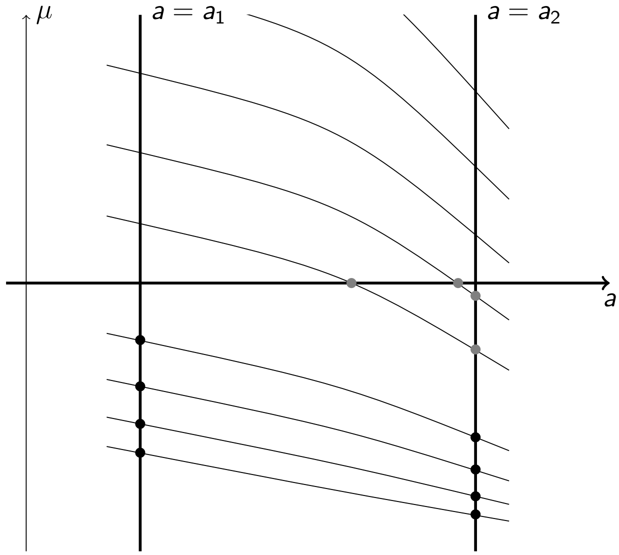

Figure 1: Diagram showing the variation of eigenvalues $\mu(a, h)$ of $P_{a,h}$ as a function of a for fixed h. The eigenvalues are strictly decreasing in a. Consequently, the number of negative eigenvalues of $P_{a_2,h}$ is equal to the number of negative eigenvalues of $P_{a_1,h}$ together with the number that cross the a-axis between $a = a_1$ and $a = a_2$.

that eigenfunctions of $P_{a,h}$ cannot vanish at the boundary. Indeed, the eigenfunctions satisfy the boundary condition $h\partial_\nu u = -au$, which shows that if u vanishes at the boundary, so does $\partial_\nu u$, which is impossible.

The eigenvalues $\mu_n(a, h)$ are thus continuous, strictly decreasing functions of a. Let $a_1 < a_2$ be real numbers. The Birman-Schwinger principle [Ivr3, Prop. 9.2.7] says that the number of negative eigenvalues of $P_{a_2,h}$ is equal to the number of negative eigenvalues of $P_{a_1,h}$, plus the number of eigenvalues $\mu_n(a, h)$ of $P_{a,h}$ that change from nonnegative to negative as a varies from a_1 to a_2. A diagram makes this clear: see Figure 1.

The strict monotonicity of $\mu(a, h)$ in a shows that the number of eigenvalues $\mu_n(a, h)$ of $P_{a,h}$ that change from nonnegative to negative as a varies from a_1 to a_2 is the same as the number of $\mu(a, h)$ (counted with multiplicity) equal to zero, for $a \in [a_1, a_2)$. Next, we observe that the space of eigenfunctions $u_n(a, h)$ of $P_{a,h}$ with zero eigenvalue, i.e. $\mu_n(a, h) = 0$ is in one-to-one correspondence with the space of eigenfunctions of $C(\lambda)$, $\lambda = h^{-1}$, with eigenvalue $(a-i)(a+i)^{-1}$, or equivalently $e^{i\theta}$ where $a = -\cot(\theta/2)$. Indeed, whenever u_n is such an eigenfunction of $P_{a,h}$, then

$$f := \frac{1}{2}(h\partial_\nu u - iu)\big|_{\partial M} \tag{2.1}$$

is an eigenfunction of $C(\lambda)$, with eigenvalue $(a-i)(a+i)^{-1}$. Conversely, if f is an eigenfunction of $C(\lambda)$ with eigenvalue $(a-i)(a+i)^{-1}$, then by definition there exists a Helmholtz function u such that u is related to f according to (2.1), and we have $(h\partial_\nu + a)u = 0$ at ∂M. This completes the proof. □

Remark 2.1. We can apply similar arguments for $\lambda^{-\delta}\rho^{-1}R(\lambda)$ as $\rho > 0$ is a smooth function on ∂M and then plug corresponding parameters in the boundary conditions coming again to equality (1.16).

We next digress to prove that the eigenvalues of $C(\lambda)$ are monotonic (that is, they move monotonically around the unit circle) in λ. This plays no role in the remainder of our proof, but is (in the authors' opinion) of independent interest.

Proposition 2.2. *The eigenvalues of $C(\lambda)$ rotate clockwise around the unit circle as λ increases.*

Remark 2.3. This implies that the eigenvalues of $R_{\mathrm{scl}}(\lambda)$ are monotone decreasing in λ.

Proof. As discussed in the previous proof, $C(\lambda)$ has eigenvalue $e^{i\theta}$ if and only if $P_{a,h}$ has a zero eigenvalue, where $a = a(\theta) = -\cot(\theta/2)$. Thus, as a function of $h = \lambda^{-1}$, $\theta(h)$ is defined implicitly by the condition

$$\mu(a(\theta), h) = 0.$$

Since a is a strictly increasing function of θ, and we have just seen that μ is a strictly decreasing function of a, it suffices to show that when $\mu = 0$, μ is a strictly increasing function of h, hence a strictly decreasing function of λ.

We now compute the derivative of μ with respect to h, at a value of a and h where $\mu(a,h)=0$. We have

$$\begin{aligned}\frac{d}{dh}\mu(a,h) &= \frac{d}{dh}((h^2\Delta-1)u(h),u(h))_M \\ &= 2h(\Delta u,u)_M + ((h^2\Delta-1)u'(h),u(h))_M + ((h^2\Delta-1)u(h),u'(h))_M \\ &= 2h(\Delta u,u)_M + ((h^2\Delta-1)u',u)_M - (u',(h^2\Delta-1)u)_M.\end{aligned}$$

In the third line, we used the fact that $(h^2\Delta-1)u=0$ when $\mu(h)=0$. Note the second term is not zero, as u' is not in the domain of the operator due to the changing boundary condition, so we cannot move the operator to the right hand side of the inner product without incurring boundary terms. We use the Gauss-Green formula to express the last two terms as a boundary integral:

$$\begin{aligned}\mu'(h) &= 2h(\Delta u,u)_M + h(h\partial_\nu u',u)_{\partial M} - h(u',h\partial_\nu u)_{\partial M} \\ &= 2h(\Delta u,u)_M + h(h\partial_\nu u',u)_{\partial M} + ha(u',u)_{\partial M}.\end{aligned}$$

Differentiating the boundary condition we find that

$$(h\partial_\nu + a)u' = -h\partial_\nu u \text{ at } \partial M.$$

Substituting that in we get

$$\mu'(h) = 2h(\Delta u,u)_M - h(u,\partial_\nu u)_{\partial M}.$$

Applying Gauss-Green again, we get

$$\begin{aligned}\mu'(h) &= h(\Delta u,u)_M + h\|\nabla u\|_M^2 \\ &= h^{-1}\left(\|u\|^2_{L^2(M)} + \|h\nabla u\|^2_{L^2(M)}\right) > 0.\end{aligned}$$

3 Semiclassical Spectral Asymptotics

In this section, we prove Theorem 1.2. Essentially, we have arrived at a rather standard semiclassical spectral asymptotics problem and results are due to [Ivr3], Chapter 5 or [Ivr4], Chapter 7. See the appendix to this paper for further discussion.

Proposition 3.1. *(i) Let* $\mathsf{N}_h^-(a)$ *be as in (1.17). The following asymptotic holds as* $h \to +0$*:*

$$\mathsf{N}_h^-(a) = (2\pi h)^{-d}\omega_d \operatorname{vol}(M) + O(h^{1-d}) \tag{3.1}$$

(ii) Further, if the set of periodic billiards on M *has measure* 0 *then as* $h \to +0$*:*

$$\mathsf{N}_h^-(a) = (2\pi h)^{-d}\omega_d \operatorname{vol}(M) + h^{1-d}\kappa(a)\operatorname{vol}'(\partial M) + o(h^{1-d}) \tag{3.2}$$

with $\kappa(a)$ *given by (1.20).*

Proof. One can check easily that the operator $P_{a,h}$ is microhyperbolic at energy level 0 at each point $(x,\xi) \in T^*M$ in the direction ξ; further, the boundary value problem is microhyperbolic at each point $(x';\xi') \in T^*\partial M$ at energy level 0 in the multidirection (ξ', ξ_1^-, ξ_1^+) with $\xi_1 = \xi_1^\pm$ roots of $\sum g^{jk}\xi_j\xi_k = 0$; finally, the boundary value problem is elliptic at each point of the elliptic zone ($\subset T^*\partial M$) if $a \le 0$, and either elliptic or microhyperbolic in the direction ξ' at each point of the elliptic zone ($\subset T^*\partial M$) if $a > 0$ — see definitions in Chapters 2, 3 of [Ivr4]. Then statements (1.18), (1.19) follow from Theorems 7.3.11 and 7.4.1 of [Ivr4].

We now assume that the set of periodic billiards on M has measure zero, and compute the second term in the spectral asymptotic explicitly. Similar calculations appear in [FG].

To do this, one can use method of freezing coefficients (see the appendix, or [Ivr4], 7.2) which results in

$$h^{1-d}\kappa(a) = \int_{\mathbb{R}^+} \bigl(e(0,x_1;0,x_1;1) - (2\pi h)^{-d}\omega_d\bigr)\,dx_1 \tag{3.3}$$

where $e(x',x_1;y',y_1;\tau)$ is the Schwartz kernel of the spectral projector $E(\tau)$ of the operator $H_a = h^2\Delta$ in half-space $\mathbb{R}^{d-1}\times\mathbb{R}^+ \ni (x',x_1)$ with domain $\mathfrak{D}(H_a) = \{u \in H^2 :\ (h\partial_{x_1} + a)u|_{x_1=0} = 0\}$.

We obtain this spectral projector by integrating the spectral measure. This in turn is obtained via Stone's formula

$$dE_L(\sigma) = \frac{1}{2\pi i}\Bigl(\bigl(L - (\sigma + i0)\bigr)^{-1} - \bigl(L - (\sigma - i0\bigr)^{-1}\Bigr)\,d\sigma. \tag{3.4}$$

Consider the resolvent for H_a, $(H_a - \sigma)^{-1}$, for $\sigma \in \mathbb{C} \setminus \mathbb{R}$. Using the Fourier transform in the x' variables, we can write the Schwartz kernel of this resolvent in the form

$$(2\pi h)^{1-d} \int e^{i(x'-y')\cdot\xi'} (T_a + |\xi'|^2 - \sigma)^{-1}(x_1, y_1)\, d\xi'. \tag{3.5}$$

Here T_a is the one-dimensional operator $T_a = -h^2\partial^2 + |\xi'|^2$ on $L^2(\mathbb{R}_+)$ under the boundary condition $(h\partial + a)u|_{x_1=0} = 0$. The spectral projector $E_{H_a}(1)$ is therefore given by

$$(2\pi h)^{1-d} \int_{-\infty}^{1} \int e^{i(x'-y')\cdot\xi'} dE_{T_a}(\sigma - |\xi'|^2)(x_1, y_1)\, d\xi'\, d\sigma. \tag{3.6}$$

Thus, we need to find the spectral measure for T_a. Write $\sigma - |\xi'|^2 = \eta^2$, where we take η to be in the first quadrant of $\mathbb{C}$ for $\operatorname{Im}\sigma > 0$, and in the fourth quadrant for $\operatorname{Im}\sigma < 0$.

Lemma 3.2. *Suppose that $\operatorname{Im}\eta > 0$ and $\operatorname{Re}\eta \geq 0$. Then the resolvent kernel $(T_a - \eta^2)^{-1}$ takes the form*

$$(T_a - \eta^2)(x, y) = \begin{cases} \frac{i}{2h\eta}\left(e^{i\eta(x-y)/h} + \frac{i\eta - a}{i\eta + a} e^{i\eta(x+y)/h}\right), & x > y \\ \frac{i}{2h\eta}\left(e^{i\eta(y-x)/h} + \frac{i\eta - a}{i\eta + a} e^{i\eta(x+y)/h}\right), & x < y. \end{cases} \tag{3.7}$$

If $\operatorname{Im}\eta < 0$ and $\operatorname{Re}\eta \geq 0$, then the resolvent kernel $(T_a - \eta^2)^{-1}$ takes the form

$$(T_a - \eta^2)(x, y) = \begin{cases} -\frac{i}{2h\eta}\left(e^{i\eta(y-x)/h} + \frac{i\eta + a}{i\eta - a} e^{-i\eta(x+y)/h}\right), & x > y \\ -\frac{i}{2h\eta}\left(e^{i\eta(x-y)/h} + \frac{i\eta + a}{i\eta - a} e^{-i\eta(x+y)/h}\right), & x < y. \end{cases} \tag{3.8}$$

Proof. In the regions $x < y$ and $x > y$, the resolvent kernel must be a linear combination of $e^{i\eta x/h}$ and $e^{-i\eta x/h}$. Moreover, for $\operatorname{Im}\eta > 0$, we can only have the $e^{+i\eta x/h}$ term, as $x \to \infty$, as the other would be exponentially increasing. So we can write the kernel in the form

$$\begin{cases} c_1 e^{+i\eta x/h}, & x > y \\ c_2 e^{+i\eta x/h} + c_3 e^{-i\eta x/h}, & x < y. \end{cases} \tag{3.9}$$

We apply the boundary condition, and the two connection conditions at $x = y$, namely continuity, and a jump in the derivative of $-1/h$, in order to obtain the delta function $\delta(x-y)$ after applying T_a. These three conditions determine the c_i uniquely, and we find that, in the case $\operatorname{Im}\eta > 0$,

$$c_1 = \frac{i}{2h\eta}\Big(e^{-i\eta y/h} + \frac{i\eta - a}{i\eta + a}e^{+i\eta y/h}\Big), \tag{3.10$_1$}$$

$$c_2 = \frac{i}{2h\eta}\frac{i\eta - a}{i\eta + a}e^{+i\eta y/h}, \qquad c_3 = \frac{i}{2h\eta}e^{+i\eta y/h}, \tag{3.10$_{2,3}$}$$

yielding (3.7). A similar calculation yields (3.8). □

We now apply (3.4) to find the Schwartz kernel of the spectral measure for T_a.

Lemma 3.3. *The spectral measure $dE_{T_a}(\tau)$ is given by the following.*

(i) For $\tau \geq 0$, $\tau = \eta^2$

$$\begin{aligned} &dE_{T_a}(\tau) \\ &= \frac{1}{4\pi h\eta}\Big(e^{i\eta(x-y)/h} + e^{i\eta(y-x)/h} + \frac{i\eta - a}{i\eta + a}e^{i\eta(x+y)/h} + \frac{i\eta + a}{i\eta - a}e^{-i\eta(x+y)/h}\Big)\, 2\eta d\eta. \end{aligned} \tag{3.11}$$

(ii) For $\tau < 0$, the spectral measure $dE(\tau)$ vanishes for $a \leq 0$, while for $a > 0$

$$dE_{T_a}(\tau) = \frac{2a}{h}e^{-ax/h}e^{-ay/h}\delta(\tau + a^2)d\tau. \tag{3.12}$$

Proof. This follows directly from Lemma 3.2 and Stone's formula, (3.4). The extra term for $a > 0$ arises from the pole in the denominator, $i\eta + a$ for $\operatorname{Im}\eta > 0$ and $i\eta - a$ for $\operatorname{Im}\eta < 0$ in the expressions (3.7), (3.8), which only occurs for $a > 0$. For τ negative, we need to set $\eta = i\sqrt{-\tau} + 0$ in (3.7) and $\eta = -i\sqrt{-\tau} + 0$ in (3.8), and subtract. Then everything cancels except at the pole, where we obtain a delta function $-2\pi i\delta(\sqrt{-\tau} - a)$, which arises from $(\sqrt{-\tau} + i0 + a)^{-1} - (\sqrt{-\tau} - i0 + a)^{-1}$. This term arises from the negative eigenvalue $-a^2$ which occurs for $a > 0$, corresponding to the eigenfunction $\sqrt{2a/h}\, e^{-ax/h}$. □

Plugging this into (3.6), and making use of the fact that $d\sigma d\xi' = 2\eta d\eta d\xi'$, we find that the Schwartz kernel of $E_{H_a}(1)$ is given by

$$(3.13)\quad (2\pi h)^{-d} \int_0^1 \int H(1 - |\xi'|^2 - \eta^2) e^{i(x'-y')\cdot\xi'} \times \left(e^{i\eta(x_1-y_1)/h} + e^{i\eta(y_1-x_1)/h} + \frac{i\eta - a}{i\eta + a} e^{i\eta(x_1+y_1)/h} + \frac{i\eta + a}{i\eta - a} e^{-i\eta(x_1+y_1)/h} \right) d\xi'\, d\eta$$

for $a \leq 0$ while for $a > 0$, it is given by the sum of (3.13) and

$$(3.14)\quad (2\pi h)^{1-d} \frac{2a}{h} e^{-ax_1/h} e^{-ay_1/h} \int_{-\infty}^1 \int e^{i(x'-y')\cdot\xi'} \delta(\sigma - |\xi'|^2 + a^2)\, d\xi'\, d\sigma.$$

We are actually interested in the value on the diagonal. Setting $x = y$, and performing the trivial ξ' integral, we find that the Schwartz kernel of the spectral projector $E_{H_a}(1)(x, x)$ on the diagonal is given by

$$(3.15)\quad \frac{\omega_{d-1}}{(2\pi h)^d} \int_0^1 (1 - \eta^2)^{(d-1)/2} \left(2 + \frac{i\eta - a}{i\eta + a} e^{2i\eta x_1/h} + \frac{i\eta + a}{i\eta - a} e^{-2i\eta x_1/h} \right) d\eta + H(a) \frac{(d-1)\omega_{d-1}}{(2\pi h)^{d-1}} \frac{a}{h} e^{-2ax_1/h} \int_{-a^2}^1 (\sigma + a^2)^{(d-3)/2}\, d\sigma.$$

Since

$$\omega_{d-1} \int_0^1 2(1 - \eta^2)^{(d-1)/2}\, d\eta = \omega_d,$$

we see by comparing with (3.3) that this term disappears in the expression for $\kappa(a)$ and we have, after performing the x_1 integral as in (3.3)

$$(3.16)\quad h^{1-d}\kappa(a) = \frac{\omega_{d-1}}{(2\pi h)^d} \int_0^1 (1 - \eta^2)^{(d-1)/2} \times \left(\frac{i\eta - a}{i\eta + a} \left(\frac{ih}{2} (\eta + i0)^{-1} \right) - \frac{i\eta + a}{i\eta - a} \left(\frac{ih}{2} (\eta - i0)^{-1} \right) \right) d\eta + H(a) \frac{(d-1)\omega_{d-1}}{2(2\pi h)^{d-1}} \int_{-a^2}^1 (\sigma + a^2)^{(d-3)/2}\, d\sigma.$$

Simplifying a bit, and performing the σ integral, we have

$$\kappa(a) = -\frac{i\omega_{d-1}}{2(2\pi)^d}\int_{-1}^{1}(1-\eta^2)^{(d-1)/2}\frac{(i\eta-a)^2}{a^2+\eta^2}(\eta+i0)^{-1}\,d\eta + H(a)\frac{\omega_{d-1}}{(2\pi)^{d-1}}(1+a^2)^{(d-1)/2}. \tag{3.17}$$

We further simplify this expression by expanding $(i\eta-a)^2 = a^2 - 2ia\eta - \eta^2$, and noting that the contribution of the $-\eta^2$ term is zero, as this gives an odd integrand in the η integral. A similar statement can be made for the a^2 term, except that there is a contribution from the pole in this case. This leads to the expression

$$\kappa(a) = \frac{\omega_{d-1}}{(2\pi)^{d-1}}\Big(-\frac{1}{2\pi}\int_{-1}^{1}(1-\eta^2)^{(d-1)/2}\frac{a}{a^2+\eta^2}\,d\eta - \frac{1}{4} + H(a)(1+a^2)^{(d-1)/2}\Big). \tag{3.18}$$

Although not immediately apparent, this formula is continuous at $a=0$. In fact, the function $a(a^2+\eta^2)^{-1}$ has a distributional limit $(\operatorname{sgn} a)\pi\delta(\eta)$ as a tends to zero from above or below. The change of sign as a crosses 0 means that the integral in (3.18) has a jump of -1 as a crosses zero from negative to positive. That exactly compensates the jump in the final term.

In odd dimensions, we can compute this integral exactly. In particular, in dimension $d=3$, we find that

$$\kappa(a) = \frac{\omega_2}{(2\pi)^2}\Big(-\frac{1}{4}+\frac{a}{\pi}+(1+a^2)\big(1-\frac{\operatorname{arccot} a}{\pi}\big)\Big). \tag{3.19}$$

Proof of Theorem 1.2. This follows immediately from Proposition 3.1 and Proposition 1.1. □

Remark 3.4. The second term of the expansion in [FG, Theorem 1.1] is obtained by computing

$$(2\pi h)^{1-d}\int_{-\infty}^{1}(1-\sigma)\int e^{i(x'-y')\cdot\xi'}\,dE_{T_a}(\sigma-|\xi'|^2)(x_1,y_1)\,d\xi'\,d\sigma \tag{3.20}$$

instead of (3.6).

4 Relation to Dirichlet Boundary Condition

In this section we observe that the limit $a \to -\infty$ corresponds to the Dirichlet boundary condition. More precisely, we have

Proposition 4.1. *Let* $\mathsf{N}_h^-(-\infty)$ *denote the limit*

$$\mathsf{N}_h^-(-\infty) := \lim_{a \to -\infty} \mathsf{N}_h^-(a),$$

where $\mathsf{N}_h^-(a)$ *is given by (1.17). Then we have*

$$\mathsf{N}_h^-(-\infty) = \#\{\lambda_j \le h^{-1} \mid \lambda_j^2 \text{ is a Dirichlet eigenvalue of } \Delta\}. \tag{4.1}$$

Remark 4.2. Because the quadratic form (1.15) is monotone in a, the counting function $\mathsf{N}_h^-(a)$ is monotone in a. Hence the limit above exists.

Proof. We use the min-max characterisation of eigenvalues. Let $\tilde{\mathsf{N}}_D(\lambda)$ denote the number of Dirichlet eigenvalues (counted with multiplicity) less than or equal to $\lambda = h^{-1}$. This is equal to the maximal dimension of a subspace of $H_0^1(M)$ on which the quadratic form Q_D, given by

$$Q_D(u, u) = h^2 \|\nabla u\|_2^2 - \|u\|_2^2 \tag{4.2}$$

is negative semidefinite. On the other hand, $\tilde{\mathsf{N}}_h^-(a)$ is equal to the maximal dimension of a subspace of $H^1(M)$ on which the quadratic form Q_a given by (1.15) is (strictly) negative definite.

We first show that $\tilde{\mathsf{N}}_D(h^{-1}) \le \tilde{\mathsf{N}}_h^-(-\infty)$. Let V be the vector space spanned by Dirichlet eigenfunctions with eigenvalue $\le \lambda^2$. Clearly, the quadratic form Q_a is negative *semi*definite on V, and if λ^2 is not a Dirichlet eigenvalue, then it is negative definite, proving the assertion. In the case that λ^2 is a Dirichlet eigenvalue, we perturb V to V_ϵ, a vector space of $H^1(M)$ of the same dimension as V, so that, for for ϵ sufficiently small depending on a, Q_a is negative definite on V_ϵ. For simplicity we only do this in the case that the λ^2-eigenspace is one dimensional, leaving the general case to the reader. To do this, we choose an orthonormal basis of V (with respect to the L^2 inner product) of Dirichlet eigenfunctions $v_1, \dots, v_k$ with eigenvalues $\lambda_1^2 \dots \lambda_k^2$, where $\lambda_k = \lambda$. Then we perturb only v_k, leaving the others fixed. We choose $s \in H_0^1(M)^\perp$, the orthogonal complement of $H_0^1(M)$ in $H^1(M)$ (with respect to the inner product in $H^1(M)$), so that

$$Q_a(v_i, s) = 0, \quad i < k \text{ and } Q_a(v_k, s) > 0. \tag{4.3}$$

We check that this is possible. Notice that $s \in H_0^1(M)^\perp$ implies that $(\Delta+1)s = 0$ in M. Then as v_i has zero boundary data, we have

$$(\lambda_i^2+1)(v_i,s)_M = (\Delta v_i, s)_M - (v_i, \Delta s)_M = \langle \partial_\nu v_i, s\rangle_{\partial M}. \tag{4.4}$$

We choose s so that $\langle \partial_\nu v_i, s\rangle_{\partial M}$ vanishes for $i < k$ and is positive for $i = k$. This is possible: in fact, due to the unique solvability of the boundary value problem

$$(\Delta+1)s = 0, \quad s|_{\partial M} = f \in H^{1/2}(M), \tag{4.5}$$

for $s \in H^1(M)$, we see that s can have any boundary value in $H^{1/2}(\partial M)$ which is dense in $L^2(\partial M)$. Then using (4.4) we see that $\langle \partial_\nu v_k, s\rangle_{\partial M} > 0$ implies that $(v_k, s)_M > 0$.

We now define V_ϵ to be the span of $v_1, \dots, v_{k-1}$ and $v_k + \epsilon s$. Then we have

$$Q_a(v_i, v_k + \epsilon s) = 0, \ \ i < k \tag{4.6}$$

and

$$\begin{aligned} Q_a(v_k+\epsilon s, v_k+\epsilon s) &= Q_a(v_k,v_k) + 2\epsilon Q_a(v_k,s) + \epsilon^2 Q_a(s,s) \\ &= 2\epsilon Q_a(v_i,s_i) + \epsilon^2 Q_a(s_i,s_i) \\ &= -2\epsilon(h^2+1)(v_i,s_i)_M + O(\epsilon^2 a^2) \end{aligned} \tag{4.7}$$

which is strictly negative for ϵa^2 small enough. It follows that Q_a is negative definite on V_k when ϵa^2 is small enough. A similar construction can be made when λ^2 has multiplicity greater than 1.

We next show that $\tilde{\mathsf{N}}_D(h^{-1}) \geq \mathsf{N}_h^-(-\infty)$. We argue by contradiction: if not, then for any a, there is a vector space W of dimension $\geq k+1$ on which Q_a is negative definite. Then there is a nonzero vector $w \in W$ orthogonal (in the $H^1(M)$ inner product) to V. We can write $w = w' + s$ where $w' \in H_0^1(M)$ and $s \in H_0^1(M)^\perp$. Then w' is a linear combination of Dirichlet eigenfunctions with eigenvalue $\geq \lambda' > \lambda$, where λ' is the smallest eigenvalue larger than λ. We then have

$$\begin{aligned} 0 > Q_a(w'+s, w'+s) &= Q_a(w',w') + 2Q_a(w',s) + Q_a(s,s) \\ &\geq (\lambda'-\lambda)\|w'\|_2^2 - 2(h^2+1)\|w'\|_2\|s\|_{L^2(M)} - ha\|s\|^2_{L^2(\partial M)}. \end{aligned} \tag{4.8}$$

However, some standard potential theory shows that $\|s\|_{L^2(M)}$ is bounded by a constant times $\|s\|_{L^2(\partial M)}$. To see this, extend M to a larger manifold $\tilde{M}$ of the same dimension, and let $G(x, y)$ be the Schwartz kernel of the inverse of $(\Delta_{\tilde{M}} + 1)^{-1}$ on $L^2(\tilde{M})$, with Dirichlet boundary conditions at $\partial\tilde{M}$. We can write s as $\int_{\partial M} d_{\nu_y} G(x, y)h(y)\, dy$ where $(1/2 + D)h = s|_{\partial M}$ and D is the double layer operator on ∂M determined by G. Standard arguments show that $(1/2 + D)$ has a bounded inverse on $L^2(\partial M)$ and $d_{\nu_y} G(x, y)$ is a bounded integral operator from $L^2(\partial M)$ to $L^2(M)$. So we can write, for $a < 0$,

$$\begin{aligned} 0 &> Q_a(w' + s, w' + s) \\ &\geq (\lambda' - \lambda)\|w'\|_2^2 - 2C(h^2 + 1)\|w'\|_2\|s\|_{L^2(\partial M)} + h|a|\|s\|^2_{L^2(\partial M)^2} \end{aligned}$$

and the RHS is clearly positive for $|a|$ large enough, giving us the desired contradiction. □

A Appendix

A.1 Standard Semiclassical Asymptotics

The proof of the standard semiclassical asymptotics (i.e. asymptotics of the number of negative eigenvalues of $H_a := h^2\Delta - 1$ with the boundary condition $(h\partial_{x_1} + a)u|_{\partial M} = 0$) is in [Ivr4], Section 8.3 and also in [Ivr3], Section 5.3, but we describe a simplified albeit less general proof. Basically it is a simplified proof of [Ivr1], used also in [LH], Section 29.3.

A.2 Tauberian Theorem

We use the following "semiclassical" version of the Tauberian theorem in [Ivr1].

Proposition A.1. *Let $e_h(\lambda)$ be an nondecreasing function of λ, depending on the parameter $h > 0$, equal to zero for $\lambda \leq \Lambda_0$. Let $\beta \in C_c^\infty(\mathbb{R})$ be a cutoff function with $\beta(t) = 1$, $|t| \leq 1/2$, $\beta(t) = 0$, $|t| \geq 1$, and $\hat{\beta}(\lambda) > 0$. Let $\beta_T(t) = \beta(t/T)$. Assume that for all λ, we have*

$$|e_h(\lambda)| \leq C'(1 + |\lambda|)^M h^{-d} \tag{A.1}$$

and, for all $\lambda \in [\Lambda_0, \Lambda_1]$ *we have*

$$\frac{1}{h}\int_{-\infty}^{\infty} \hat{\beta}_T\Big(\frac{\lambda-\mu}{h}\Big)\, de_h(\mu) = A_0(\lambda)h^{-d} + A_1(\lambda)h^{1-d} + o(h^{1-d}), \quad h \to 0. \tag{A.2}$$

Then for all $\lambda \in [\Lambda_0, \Lambda_1 - \epsilon]$ *we have*

$$\Big| e_h(\lambda) - B_0(\lambda)h^{-d} - B_1(\lambda)h^{1-d} \Big| \le \frac{C\|A_0\|_{L^\infty([\Lambda_0,\Lambda_1])}}{T} h^{1-d} + o(h^{1-d}), \tag{A.3}$$

where

$$B_i(\lambda) = \int_{-\Lambda_0}^{\lambda} A_i(\mu)\, d\mu$$

and C *depends only on* ϵ, Λ_1, C' *and* β.

This is proved by modifying the proof of the corresponding proposition in [Shub], pp 152-153.

A.3 Propagator

We now fix $a \in \mathbb{R}$ and let $e_h(\lambda)$ be the number of eigenvalues, counting multiplicity, of the operator $P_{a,h}$ that are less than λ, or equivalently, the trace of the spectral projection $E_{a,h}(\lambda)$ for $P_{a,h}$. According to Proposition A.1, it suffices to consider the smoothed spectral projector,

$$\mathrm{Tr}\Big(\frac{1}{h}\int_{-\infty}^{\infty} \hat{\beta}\Big(\frac{\lambda-\mu}{h}\Big)\, dE_{a,h}(\mu)\Big), \tag{A.4}$$

since it is straightforward to show that the estimate (A.1) holds with $M = d$. By the spectral theorem, this is precisely the trace of the operator

$$\mathrm{Tr}\Big(\hat{\beta}\Big(\frac{\lambda - P_{a,h}}{h}\Big)\Big). \tag{A.5}$$

If we are only interested in this for λ in some interval $[\Lambda, \Lambda_1]$, then, up to $O(h^\infty)$ errors we can compose with a smooth function $\phi(P_{a,h})$ where $\phi \in C_c^\infty(\mathbb{R})$, and $\phi = 1$ on $[\Lambda - \epsilon, \Lambda_1 + \epsilon]$. Then, using the Fourier transform we can express this operator in terms of the propagator $e^{itP_{a,h}/h}$:

$$\int_{-\infty}^{\infty} e^{-it\lambda/h}\beta(t)\phi(P_{a,h})e^{itP_{a,h}/h}\, dt. \tag{A.6}$$

Since $(hD_t - P_{a,h})e^{itP_{a,h}/h} = 0$, this is the same as

$$\int_{-\infty}^{\infty} e^{-it\lambda/h}\beta(t)\phi(hD_t)e^{itP_{a,h}/h}\,dt. \tag{A.7}$$

The advantage of the spectral cutoff $\phi(hD_t)$ is that the operator $\phi(hD_t)e^{itP_{a,h}/h}$ has finite speed of propagation.

A.4 Propagation of Singularities

Let $u_h(x,y,t)$ be the Schwartz kernel of $e^{ih^{-1}tP_{a,h}}$; then $u_h(x,y,t) = u_h^0(x,y,t) + u_h^1(x,y,t)$ where $u_h^0(x,y,t)$ is a free space solution and $u_h^1(x,y,t)$ satisfies

$$(hD_t - P_{a,h})u^1 = 0, \quad u^1|_{t=0} = 0, \quad (hD_{x_1} + a)(u^0 + u^1)|_{\partial M} = 0. \tag{A.8}$$

We define

$$\sigma_h^i(t) := \int_M \phi(hD_t)u^i(x,x,t)\,dx, \quad i = 0, 1. \tag{A.9}$$

We claim that, for suitable ϕ, $\sigma_h^i(t)$ has an isolated singularity (in the semiclassical sense of nontrivial behaviour as $h \to 0$) at $t = 0$. More precisely, we claim that if $\phi \in C^\infty$ and is supported in $(-\epsilon_0, \epsilon_0)$, then

$$\sigma_h^i(t) = O(h^\infty) \text{ for } \epsilon \le |t| \le \epsilon_0, \tag{A.10}$$

where ϵ_0 is a fixed, sufficiently small constant, and $0 < \epsilon < \epsilon_0$ is arbitrary.

This follows from propagation of singularities arguments. The bicharacteristic flow for $P_{a,h}$ is given by

$$\begin{cases} \dot{t} = 1, \\ \dot{\tau} = 0, \\ \dot{x}^i = 2g^{ij}(x)\xi_j, \\ \dot{\xi}_j = -2\dfrac{\partial g^{kl}}{\partial x^j}\xi_k\xi_l. \end{cases} \tag{A.11}$$

That is, with respect to the parameter t, (x,ξ) moves along a geodesic at speed $2|\xi|_g$, and τ is fixed. By standard propagation of singularities arguments, the (semiclassical) wavefront set of u^0 is contained in the conormal bundle of $\{t = 0, s = y\}$ together with the forward bicharacteristic flow from this conormal bundle intersected with the characteristic variety of $hD_t - P_{a,h}$, namely $\{\tau = |\xi|_g^2 - 1\}$. Composing with $\phi(hD_t)$ restricts this wavefront set to be contained in $\{\tau \in (-\epsilon_0, \epsilon_0)\}$. That implies that $\big||\xi|_g - 1\big| \le 2\epsilon_0$. So for small time, the wavefront set of u_0 is restricted to the set where $|d(x,y) - 2t| \le 2\epsilon_0 t$. In particular, points with $x = y$ are not in the wavefront set for t in a deleted neighbourhood of 0. This proves (A.10) for $i = 0$.

A similar argument for u^1 shows that $\phi(hD_t)u^1(t,x,y)$ is $O(h^\infty)$ for $|t| \le \epsilon_0$ unless we have

$$\mathrm{dist}(x, \partial M) + \mathrm{dist}(y, \partial M) \le 2\epsilon_0(1 + 2\epsilon_0).$$

Thus, we can work in a collar neighbourhood of ∂M. We can choose coordinates $x = (x_1, x')$ so that the boundary is given by $x_1 = 0$, $x_1 \ge 0$ on M, and the metric takes the form $dx_1^2 + g'_{ij}(x_1, x')x'^i x'^j$, that is, Fermi coordinates near the boundary. Now we split the analysis of u^1 into two cases. We write the identity operator in the x' coordinates in the form $\mathrm{Id} = Q_{\mathrm{norm}} + Q_{\tan}$, where Q_* are pseudodifferential operators in the x' variables such that the symbol q_{norm} of Q_{norm} is supported in $\{|\xi'| \le 2\epsilon_1\}$ and $q_{\tan}$ is supported in $\{|\xi'| \ge \epsilon_1\}$.

Correspondingly, write

$$\phi(hD_t)u^1 = \phi(hD_t)Q_{\tan}(x', hD_{x'})u^1 + \phi(hD_t)Q_{\mathrm{norm}}(x', hD_{x'})u^1.$$

For the first term, a standard positive commutator argument in the x' variables only shows that this term is $O(h^\infty)$ unless $\mathrm{dist}(x', y') \ge 2\epsilon_1 t - \epsilon'$ for arbitrary $\epsilon' > 0$; in particular, if $x' = y'$ then this is $O(h^\infty)$ for $t \ge \epsilon$, $\epsilon > 0$ arbitrary. On the other hand, for the Q_{norm} term, then we have $\xi_1^2 = 1 + O(\epsilon_0 + \epsilon_1)$. In particular, this means that $\dot{x}_1 = 1 + O(\epsilon_0 + \epsilon_1)$, so the propagation is transverse (in fact, nearly normal) to ∂M. A standard propagation of singularities argument shows that the wavefront set of $\phi(hD_t)Q_{\mathrm{norm}}u^1$ for $\epsilon \le |t| \le \epsilon_0$ is contained in

$$\begin{aligned}\mathrm{WF}_h(\phi(hD_t)Q_{\mathrm{norm}}u^1) &\cap \{x = y,\ \epsilon \le |t| \le \epsilon_0\} \\ &\subset \big\{(t, x, x; \tau, \xi, \eta) \mid \xi_1, \eta_1 = 1 + O(\epsilon_0 + \epsilon_1)\big\},\end{aligned}$$

since the only way to have $x = y$ is to bounce off the boundary, in which case ξ_1, the momentum in the normal direction, changes from being approximately opposite to η_1 to being approximately equal. This wavefront set is killed under restriction to $x = y$ and then integration in x, showing that $\phi(hD_t)Q_{\mathrm{norm}}u^1$ is also $O(h^\infty)$ for $\epsilon \le |t| \le \epsilon_0$. This establishes (A.10).

A.5 Method of Successive Approximations

We now observe that (A.10) self-improves to the statement that

$$\sigma_h^i(t) = O(h^\infty) \text{ for } h^{1-\delta} \le |t| \le \epsilon_0, \quad \delta > 0. \tag{A.12}$$

This follows from a simple scaling argument. Fix a base point $y \in \partial M$, and consider the scaled metric (following [Mel])

$$g_{T,y} = g_{ij}(TX + y)dX^i dX^j$$

where T is a small parameter. Let $u_{T,\hbar}(t, X)$ be given by

$$u_{T,\hbar}(t, X) = T^{d+1}\big(\phi(hD_t)u_{T\hbar}\big)(Tt, y + TX, y);$$

then, with $\hbar := h/T$ we have

$$\begin{aligned}\left(\hbar D_t - \hbar^2\Delta_{g_{T,y}}\right)&u_{T,\hbar}(t, X) = \\ &T^{(d+1)}\left(hD_t - h^2\Delta_g\right)u_h(Tt, y + TX, y) = \phi(hD_t)\delta(t)\delta(X),\end{aligned} \tag{A.13}$$

$$(\hbar\partial_{X_1} + a)u_{T,\hbar}(t, X) = 0, \quad X_1 = 0. \tag{A.14}$$

Using (A.10) we see that we have

$$\int_M \phi(\hbar D_t)u_{T,\hbar}(X, X, t)\, dX = O(T^{-(d+1)}h^\infty) \text{ for } \epsilon \le |t| \le \epsilon_0, \tag{A.15}$$

In particular, (A.15) is $O(h^\infty)$ provided that $T \ge h^{1-\delta}$ for arbitrary $\delta > 0$. Unravelling the scaling demonstrates (A.12).

Therefore if we want to construct $\sigma(t)$ for $|t| \le \epsilon_0$ it suffices to construct it for $|t| \le t_* = h^{1-\delta}$. However on this short interval we can construct it by the method of successive approximations. For each $y \in M$ we let P_y be the constant coefficient differential operator $P_{a,h}$ with coefficients frozen at y. Then we regard $P_{h,a}$ as a perturbation of P_y for x close to y. So $K = P_{h,a} - P_y$ is a second order differential operator with coefficients that are $O(x-y)$. The perturbation K is $O(t_*)$ due to finite speed of propagation and each successive term in the approximation acquires a factor not exceeding $Ct_* \cdot t_*/h = Ct_*^2 h$ due to Duhamel's principle. So the construction works for $t_* \le h^{\frac{1}{2}+\delta}$.

If we apply this to the u^0 term then the calculation proceeds as follows. We let $\overline{u^0}$ denote the propagator for the constant coefficient operator P_y with coefficients frozen at $y \in M$ (and taking only the second order derivatives). Then, with E the forward fundamental solution for P_y, we obtain a formula

$$u^0 = \overline{u^0} + EKu^0,$$

leading to a formal series

$$u^0 = \sum_{k=0}^{m} (EK)^k \overline{u^0} + (EK)^{m+1} u^0. \tag{A.16}$$

Applying the Fourier transform in x, we find that the first term is

$$\phi(hD_t)\overline{u^0} = (2\pi h)^{-d} \int e^{i(x-y)\cdot\xi/h} e^{it(|\xi|^2-1)/h} \phi(|\xi|^2 - 1)\, d\xi.$$

If we then plug this term into (A.7) then we find that this term is h^{-d} times a smooth function of λ and a. The method of successive approximations then generates a series of the form $\sum_{n=1}^{\infty} \kappa'_n(a,\lambda) h^{-d+n}$, and the terms corresponding to odd n are given by the integral in ξ of an odd function of ξ, hence vanish.

Using this expansion of u^0, we compute a series for u^1. In this case, the leading term $\overline{u^1}$ is given as follows:

$$\phi(hD_t)\overline{u^1} = (2\pi h)^{-d} \int e^{-i(x_1+y_1)\xi_1/h} e^{i(x'-y')\cdot\xi'/h} e^{it(|\xi|^2-1)/h} \phi(|\xi|^2 - 1)\, \frac{i\xi_1 + a}{i\xi_1 - a} d\xi.$$

We can form a similar formal series for u^1, which converges when $t \le h^{1/2+\delta}$. As with the case of u^0, we can check that the successive terms in the approximation for u^1, when plugged into (A.7), give a series with the contribution of $\phi(hD_t)\overline{u^1}$ at order h^{1-d} and with successive terms contributing at increasing integer powers of h.

Now, using this together with the Tauberian theorem, Proposition A.1, shows that we get a leading Weyl asymptotic with remainder term $O(h^{1-d})$, as in (1.18).

A.6 Two Term Expansion

If we assume that the measure of periodic generalized bicharacteristics is zero, then we can use the standard method to obtain a two-term expansion of the counting function. We briefly recall here the argument, following [Ivr1].

Let $\epsilon > 0$ be given. Then we decompose the identity operator on $L^2(M)$ as a sum of three terms. The first is multiplication by a cutoff function ζ identically 1 near ∂M and supported in a collar neighbourhood of ∂M, such that

$$\int_M \zeta^2 \leq \epsilon.$$

The second and third are pseudodifferential operators chosen as follows. With $T > 1$ a large constant to be chosen later, we let Λ_T denote the union of points in

$$\{(x, \xi) \in T^*M \mid |\xi|_g \in (1 - \epsilon_0, 1 + \epsilon_0)\}$$

which are either periodic with period $\leq T$ under generalized bicharacteristic flow (for $P_{a,h}$), or for which the generalized bicharacteristic of length T in both directions are not transverse to the boundary. This is a closed set of measure zero so one can find two open sets U_1, U_2 such that $T^*M = U_1 \cup U_2$, $\Lambda_T \subset U_1$, and the measure of U_1 is less than ϵ. Then we choose (semiclassical) pseudodifferential operators Q_1, Q_2 such that Q_i is microsupported in the conic set determined by U_i, and such that $\mathrm{Id} = \zeta^2 + Q_1^* Q_1 + Q_2^* Q_2$. We then define

$$\begin{aligned} e_h^0(\lambda) &= \operatorname{Tr} \zeta^2 E_{h,a}(\lambda) = \operatorname{Tr} \zeta E_{h,a} \zeta \\ e_h^i(\lambda) &= \operatorname{Tr} Q_i^* Q_i E_{h,a}(\lambda) = \operatorname{Tr} Q_i E_{h,a}(\lambda) Q_i^*, \quad i = 1, 2; \end{aligned}$$

notice that each of these is nondecreasing in λ, and the sum of the three terms is equal to the counting function for $P_{h,a}$. Correspondingly, we break (A.7) into a sum of three terms, with $i = 0, 1, 2$.

Using the series for u^0 and u^1 sketched above, we compute expansions for the three terms. Applying Proposition A.1 we find that

$$\left| e_h^0(\lambda) - A_0^0(\lambda) h^{-d} - A_1^0(\lambda) h^{1-d} \right| = O(\epsilon h^{1-d}),$$

since in this case $A_0^0(\lambda)$ is $O(\epsilon)$, as it is proportional to $\int_M \zeta^2$. For the term $i = 1$ we similarly find that

$$\left| e_h^1(\lambda) - A_0^1(\lambda) h^{-d} - A_1^1(\lambda) h^{1-d} \right| = O(\epsilon h^{1-d}),$$

since $A_0^1(\lambda)$ is proportional to the integral of $|\sigma(Q_1)|^2$ which is also $O(\epsilon)$. For the third term, we scale β to β_T, exploiting the condition that on the microsupport of Q_2, there are no periodic bicharacteristics up to time T, hence the trace of $\phi(hD_t) e^{itP_{a,h}/h}$ has no singularities for $t \in [-T, T]$ except at $t = 0$. Hence this term also has an expansion in powers of h, and we find that

$$\left| e_h^2(\lambda) - A_0^2(\lambda)h^{-d} - A_1^2(\lambda)h^{1-d} \right| = O(\frac{h^{1-d}}{T}).$$

Choosing T sufficiently large, this is also $O(\epsilon h^{1-d})$, and we have shown the existence of a two-term expansion.

It only remains to identify the first two terms. But once we know that there *is* a two-term expansion, we can identify the coefficients from the first two terms in the expansion of $\mathrm{Tr}\, \phi(hD_t)e^{itP_{a,h}/h}$ at $t = 0$. From the method of successive approximations we see that these terms arise from the contribution of $\overline{u^0}$ and $\overline{u^1}$. We observe that $\overline{u^0} + \overline{u^1}$ gives precisely the propagator for the $h^2\Delta_{\mathbb{R}^d_+}$, the flat Laplacian on the half-space $\mathbb{R}^d_+ = \{x_1 \geq 0\}$, with the boundary condition $(h\partial_{x_1} + a)\overline{u}(x, y, t) = 0$ at $x_1 = 0$. It follows that the local densities for each term of the two-term expansion is equal to the local density for the flat half-space model. This justifies the calculations in Section 3 based on this flat model.

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Spectral asymptotics for fractional Laplacians*,†

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Abstract

In this article we consider fractional Laplacians which seem to be of interest to probability theory. This is a rather new class of operators for us but our methods works (with a twist, as usual). Our main goal is to derive a two-term asymptotics since one-term asymptotics is easily obtained by R. Seeley's method.

In this article we consider fractional Laplacians. This is a rather new class of operators for us but our methods works (with a twist, as usual). Our main goal is to derive a two-term asymptotics since one-term asymptotics is rather easily obtained by R. Seeley's method.

1 Problem Set-up

Let us consider a bounded domain $X \subset \mathbb{R}^d$ with the smooth boundary $\partial X \in \mathscr{C}^\infty$ [1]. In this domain we consider a fractional Laplacian $\Lambda_m = (\Delta^{m/2})_{\mathfrak{D}}$ with $m > 0$ originally defined on functions $u \in \mathscr{C}^\infty(\mathbb{R}^d) : \theta_X u \in \mathscr{H}^{m/2}(\mathbb{R}^d)$ by

$$\Lambda_{m,X} \coloneqq (\Delta^{m/2})_{\mathfrak{D}} u = R_X \Delta^{m/2}(\theta_X u) \tag{1.1}$$

where θ_X is a characteristic function of X, R_X is an operator of restriction to X and $\Delta^{m/2}$ is a standard pseudodifferential operator in $\mathbb{R}^d$ with the Weyl symbol $g(x,\xi)^{m/2}$ where as usual $g(x,\xi)$ is non-degenerate Riemannian metrics.

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[1] Alternatively consider a bounded domain X on the Riemannian manifold $\mathcal{X}$.

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Remark 1.1. (i) We consider $\Lambda_{m,X}$ as an unbounded operator in $\mathscr{L}^2(X)$ with domain $\mathfrak{D}(\Lambda_{m,X}) = \{u \in \mathscr{L}^2(\mathbb{R}^d) : \operatorname{supp}(u) \subset \bar{X}, R_X\Lambda_m \in \mathscr{L}^2(X)\} \subset \mathscr{H}_0^{m/2}(X)$.

(ii) This operator can also be introduced through positive quadratic form with domain $\{u \in \mathscr{H}^m(\mathbb{R}^d), \operatorname{supp}(u) \subset \bar{X}\}$ and is a positive self-adjoint operator which is Friedrichs extension of operator originally defined on $\mathscr{H}_0^m(X)$.

(iii) We can consider this operator as a bounded operator from $\mathscr{H}_0^{m/2}(X)$ to $\mathscr{H}^{-m/2}(X) \coloneqq \mathscr{H}_0^{m/2\,*}(X)$.

(iv) Let $0 < m \notin 2\mathbb{Z}$. Then $\mathfrak{D}(\Lambda_{m,X}) \subset \mathscr{H}^m(X)$ if and only if $m \in (0,1)$; otherwise even eigenfunctions of $\Lambda_{m,X}$ may not belong to $\mathscr{H}^m(X)$.

(v) Since Λ_m does not possess transmission property for $m \notin 2\mathbb{Z}$, we are not in the framework of the Boutet-de-Monvel algebra, but pretty close: Λ_m possess μ-transmission property introduced by L. Hörmander and systematically studied by G. Grubb in [5, 6]. We provide definition in Subsection A.2.

We are interested in the asymptotics of the eigenvalue counting function $\mathsf{N}(\lambda)$ for $\Lambda_{m,X}$ as $\lambda \to +\infty$.

2 Preliminary Analysis

As usual we reduce problem to a semiclassical one. Let $A = A_h \coloneqq h^m\Lambda_{m,X} - 1$ with $h = \lambda^{-1/m}$, $e_h(x, y, \tau)$ the Schwartz kernel of $\theta(\tau - A_h)$ a spectral projector of A_h, and N_h^- the number of negative eigenvalues of A_h.

Proposition 2.1. *Let $\bar{x} \in X$, $B(\bar{x}, 2\gamma) \subset X$, $\gamma \geq h$. Then*

$$|e_h(x,x,0) - \mathsf{Weyl}(x)| \leq Ch^{1-d}\gamma^{-1} \qquad \forall x \in B(\bar{x},\gamma) \tag{2.1}$$

and

$$|\int \psi((x-\bar{x})/\gamma)\Bigl(e_h(x,x,0) - \mathsf{Weyl}(x)\Bigr)\,dx| \leq Ch^{1-d}\gamma^{d-1}\bigl(\gamma^{\delta} + h^{\delta}\gamma^{-\delta}\bigr) \tag{2.2}$$

as $\psi \in \mathscr{C}_0^\infty(B(0,1))$ *and* $\delta > 0$*, where*

$$\mathsf{Weyl}(x) = (2\pi h)^{-d} \operatorname{mes}(\{\xi\colon g(x,\xi) \le 1\})$$

is the standard pointwise Weyl expression.

Proof. Estimate (2.1) is easily proven by just rescaling as modulo $O(h^s\gamma^{-s})$ we get a $\hbar$-pseudodifferential operator with $\hbar = h\gamma^{-1}$.

Estimate (2.2) is easily proven by rescaling plus R. Seeley's method as described in Subsection 7.5.1 of [9]. We leave easy details to the reader. □

Then we immediately arrive to

Corollary 2.2. *(i) Contribution of the inner zone* $\{x : \operatorname{dist}(x, \partial X) \ge h\}$ *to the Weyl remainder does not exceed* Ch^{1-d}*.*

(ii) Contribution of the intermediate strip $\{x : \varepsilon \ge \operatorname{dist}(x, \partial X) \ge \varepsilon^{-1}h\}$ *to the Weyl remainder does not exceed* $\eta(\varepsilon)h^{1-d}$ *with* $\eta(\varepsilon) \to 0$ *as* $\varepsilon \to 0$*.*

Here and in what follows $\varepsilon > 0$ is an arbitrarily small constant.

Proposition 2.3. *The following estimate holds:*

$$|e_h(x,x,0)| \le Ch^{-d}. \tag{2.3}$$

Proof. The standard proof we leave to the reader. □

Theorem 2.4. *(i) For operator* A *the Weyl remainder in the asymptotics for* N_h^- *does not exceed* Ch^{1-d}*.*

(ii) For operator $\Lambda_{m,X}$ *the following asymptotics holds*

$$\mathsf{N}(\lambda) = \kappa_0\lambda^{\frac{d}{m}} + O(\lambda^{\frac{d-1}{m}}) \qquad \textit{as}\ \ \lambda \to +\infty, \tag{2.4}$$

where $\kappa_0 = (2\pi)^{-d}\varpi_d \operatorname{vol}(X)$*,* ϖ_d *is a volume of the unit ball in* $\mathbb{R}^d$ *and* $\operatorname{vol}(X)$ *means the Riemannian volume of* X*.*

Proof. Statement (i) follows immediately from Corollary 2.2(i) and Proposition 2.3. Statement (ii) follows immediately from (i) as $d \ge 2$. □

Remark 2.5. (i) Therefore, we extended the result, well-known for $m \in 2\mathbb{Z}^+$ to $m \in \mathbb{R}^+$.

(ii) This was easy but to recover the second term (which is also known for $m \in 2\mathbb{Z}^+$ under non-periodicity condition) is a much more daunting task requiring first to improve the contribution of the *near boundary strip* $\{x:\, \mathsf{dist}(x,\partial X)\le \varepsilon^{-1}h\}$ and also of the *inner zone* $\{x:\, \mathsf{dist}(x,\partial X)\ge \varepsilon\}$.

3 Propagation of Singularities near the Boundary

Without any loss of the generality one can assume that

$$X=\{x:\, x_1>0\},\qquad g^{jk}=\delta_{1j}\quad \forall j=1,\dots,d. \tag{3.1}$$

First let us study the propagation of singularities along the boundary:

Theorem 3.1. *On the energy level* $\tau: |\tau|\le \epsilon_0$

(i) Singularities (with respect to x'*) propagate with the speed not exceeding* c *with respect to* (x,ξ')*.*

(ii) For $|\xi'|\asymp\rho\ge Ch^{\frac12-\delta}$*, and* $|t|\le T=\epsilon\rho$*, singularities (with respect to* x'*) move from* $x'=y'$ *with the speed* $\asymp\rho$ *with respect to* x*.*

Proof. In the terminology of [9] both statements mean that $u=u_h(x,y,t)$, the Schwartz kernel of $e^{-ih^{-1}tA}$, satisfies

$$F_{t\to h^{-1}\tau}\chi_T(t)Q_{1,x}u\,{}^t\!Q_{2,y}=O(h^s), \tag{3.2}$$

where $F_{t\to h^{-1}\tau}$ is h-Fourier transform, $Q_1=q_1(x,hD')$ and $Q_2=q_2(x,hD')$ are h-pseudodifferential operators, ${}^t\!Q_{2,y}$ is a dual operator, acting with respect to y (and we write it to the right of the function, it is applied to), $\chi_T(t)=\chi(t/T)$, where

(a) in the Statement (i) $h^{\frac12-\delta}\le T_0$, T_0 is the small constant, the distance between $\mathsf{supp}(q_1)$ and $\mathsf{supp}(q_2)$ is at least cT, and $\chi\in\mathscr{C}_0^\infty([-1,1])$.

(b) in the Statement (ii) the diameter of $\mathsf{supp}(q_1)\cup\mathsf{supp}(q_2)$ is does not exceed $\epsilon\rho$, ϵ is the small constant, and $\chi\in\mathscr{C}_0^\infty([-1,-\frac12]\cup[\frac12,1])$;

s is an arbitrarily large exponent, $\delta > 0$ is arbitrarily small,

The proof is standard, by means of the positive commutator method, like those proofs in the Chapters 2 and 3 of [9], since it involves only pseudodifferential operators $q_j(x, hD')$ and their commutators with A, but one can see easily that those commutators do not bring any troubles as the energy level is $\asymp 1$. We leave all easy details to the reader. $\square$

Corollary 3.2. *(i) Let $\rho \geq Ch^{\frac{1}{2}-\delta}$, $h^{1-\delta} \leq \gamma \leq \epsilon$. Then the contribution of the zone $\{(x, \xi') :\, x_1 \leq \gamma, |\xi'| \asymp \rho\}$ to the Tauberian remainder with $T \in (T_*(\rho), T^*(\rho))$, where $T_*(\rho) = h^{1-\delta}\rho^{-2}$, $T^*(\rho) = \epsilon\rho$ does not exceed*

$$C\rho^{d-1}h^{-d} \times \gamma \times h^{1-\delta}\rho^{-2} \times \rho^{-1}. \tag{3.3}$$

(ii) The total contribution of the zone $\{(x, \xi') :\, x_1 \leq \gamma = h^{1-\delta}\}$ to the Tauberian error with $T = h^{1-3\delta}$ does not exceed $Ch^{-d+1+\delta}$.

Proof. In the terminology of [9] the *Tauberian error* is the difference between N^-_h and the *Tauberian expression*

$$\mathsf{N}^{\mathsf{T}}_h := h^{-1} \int_{-\infty}^{0} \Bigl(\int F_{t\to h^{-1}\tau} \bar{\chi}_T(t) u(x, x, t)\, dx \Bigr)\, d\tau, \tag{3.4}$$

where $\bar{\chi} \in \mathscr{C}_0^\infty([-1, 1])$, $\bar{\chi} = 1$ on $[-\frac{1}{2}, \frac{1}{2}]$.

The easy and standard proof of Statement (i) is left to the reader; it is like those proofs in Chapter 7 of [9].

Then the contribution of the zone $x_1 \leq h^{1-\delta}$, $|\xi'| \geq Ch^{\delta}$ to the Tauberian error with $T = h^{1-3\delta}$ does not exceed $Ch^{-d+1+\delta}$. Since the contribution of the zone $\{(x, \xi') :\, x_1 \leq \gamma = h^{1-\delta}, |\xi'| \leq Ch^{2\delta}\}$ to the asymptotics does not exceed $C\rho^{d-1}h^{-d} \times \gamma \leq Ch^{-d+1+\delta}$ we arrive to Statement (ii). $\square$

Therefore in this zone $\{(x, \xi') :\, x_1 \leq \gamma = h^{1-\delta}\}$ all we need is to pass from the Tauberian expression to the Weyl expression.

However the inner zone should be reexamined and we need to describe what happens with the propagation along Hamiltonian trajectory in the zone $\{(x, \xi) :\, x_1 \leq h^{1-\delta}\}$. We can assume that $|\xi_1| \geq \varepsilon$ since the measure of the remaining trajectories is small, here $\varepsilon > 0$ is an arbitrarily small constant.

4 Reflection of Singularities from the Boundary

4.1 Toy-Model

We start from the pilot-model which will be used to prove the main case. Namely, let us consider 1-dimensional operator on half-line $\mathbb{R}^+$ with Euclidean metrics

$$B := B_{m,a,h} = ((h^2D_x^2 + a^2)^{m/2})_{\mathfrak{D}} \tag{4.1}$$

with $a \ge 0$. We denote $\mathbf{e}_{m,a,h}(x_1, y_1, \tau)$ the Schwartz kernel of its spectral projector.

Observe that scaling $x \mapsto x\gamma^{-1}$, $\tau \mapsto \tau\rho^{-m}$ transforms operator to one with $h \mapsto h/(\rho\gamma)$, $\tau \mapsto \tau\rho^{-m}$; because of this we can assume that $h = 1$ and the second scaling implies that we can assume that either $a = 1$ or $\tau = 1$.

Proposition 4.1. *(i) The spectrum of operator $\Lambda_{m,a}$ is absolutely continuos and it coincides with $[a^m, \infty)$.*

(ii) The following equalities hold:

$$\begin{multline}\mathbf{e}_{m,a,h}(x, y, \lambda) = \mathbf{e}_{m,1,ha^{-1}}(ax, ay, \lambda a^{-m}) = \\ \lambda^{1/m}\mathbf{e}_{m,a\lambda^{-1/m},h}(\lambda^{1/m}x, \lambda^{1/m}y, 1) = a\mathbf{e}_{m,1,h}(ax, ay, \lambda a^{-m}).\end{multline} \tag{4.2}$$

Proposition 4.2. *Let $\psi \in \mathscr{C}_0^\infty([-1, 1])$, $\psi_\gamma(x) = \psi(x/\gamma)$ and $\phi \in \mathscr{C}_0^\infty([-1, 1])$, $0 \le a \le 1 - \epsilon_0$. Then as $\gamma \ge h^{1-\delta}$, $T \ge C_0\gamma$, $h^\delta \ge \eta \ge h^{1-\delta}T^{-1}$*

$$\|\phi(\eta^{-1}(hD_t - 1))\psi_\gamma e^{i(mh)^{-1}tB}\psi_\gamma|_{t=T}\| \le CT^{-1}\gamma + Ch^{\delta'}. \tag{4.3}$$

Proof. Observe first that if for u supported in $\mathbb{R}^+$ and $L = x_1hD_1 - ih/2 = L^*$

$$\operatorname{Re} i(BLu, u) = \frac{1}{2}(i[B, L]u, u), \tag{4.4}$$

and then

$$\operatorname{Re}(Lu, u_t - ih^{-1}Bu) = \frac{1}{2}(ih^{-1}[B, L]u, u) + \frac{1}{2}\partial_t \operatorname{Re}(Lu, u) \tag{4.5}$$

and

$$\operatorname{Re}(ktu + Lu, u_t - ih^{-1}Bu) = \frac{1}{2}\partial_t\bigl(kt\|u\|^2 + (Lu,u)\bigr) + \frac{1}{2}\bigl((ih^{-1}[B,L]u,u) - k\|u\|^2\bigr). \tag{4.6}$$

Let us plug

$$u = \phi(\eta^{-1}(hD_t - 1))e^{ih^{-1}TB}\psi_\gamma v \tag{4.7}$$

with $\|v\| = 1$. Then the left hand expression in (4.6) is 0 and

$$\frac{1}{2}\partial_t\bigl(kt\|u\|^2 + (Lu,u)\bigr) \le \frac{1}{2}\bigl(-(ih^{-1}[B,L]u,u) + k\|u\|^2\bigr). \tag{4.8}$$

Let us estimate from above the right-hand expression; obviously

$$ih^{-1}[B_m, L] = m(B_m - a^2 B_{m-2}). \tag{4.9}$$

(a) Assume first that $m > 2$. Then since

$$(1 - C\eta)\|u\| \le \|B_m u\| \le (1 + C\eta)\|u\| \tag{4.10}$$

due to cutoff by ϕ and

$$B_{m-2} \le B_m^{(m-2)/m} \tag{4.11}$$

in virtue of Corollary A.2 we conclude that as $k = m(1 - a^2)$ the right-hand expression does not exceed $C\eta$ and therefore

$$m(1 - a^2)t\|u\|^2 + (Lu,u) \le C\gamma + C\eta T \tag{4.12}$$

since the value of the left-hand expression as $t = 0$ does not exceed $C\gamma$.

Further, observe that on the energy levels from $(1 - C_0\eta, 1 + C_0\eta)$ the singularities propagate with a speed (with respect to x_1) not exceeding $m(1 - a^2)^{\frac{1}{2}}(1 + C_0\eta)$. Therefore we conclude that u is negligible as $|x_1| \ge m(1 - a^2)^{\frac{1}{2}}(1 + C_0\eta)T + C\gamma$ and therefore since

$$\|D_1 u\| \le (B_2 u, u) \le ((1 - a^2)^{\frac{1}{2}} + C_0\eta), \tag{4.13}$$

we conclude using (4.10) and (4.11) that

$$|(Lu,u)| \le m(1 - a^2 + C_0\eta)T + C\gamma - \epsilon_0 T\|\psi_\gamma(x_1)u\|^2 \tag{4.14}$$

and the left-hand expression of (4.12) is greater than $\epsilon_0 T\|\psi_\gamma u\|^2 - C(\eta T + \gamma)$ and we arrive to (4.3).

(b) Assume now that $0 < m < 2$. Then our above proof fails short in both estimating $\operatorname{Re} ih^{-1}([B, L]u, u)$ from below and $|(Lu, u)|$ from above and we need to remedy it.

Note first that away from $x_1 = 0$ only symbols are important and therefore the right-hand expression of (4.8) does not exceed $\frac{m}{2}(a^m - a^2)\|\psi_\sigma u\|^2 + Ch^2\sigma^{-2}$ since $\|B_{m-2}\| \le a^{m-2}$. Indeed, we need just to decompose $1 = \psi_\sigma^2 + \psi_\sigma'^2$ and use our standard arguments to rewrite the right-hand expression of (4.8) as the sum of the same expressions for $\psi_\sigma u$ and $\psi'_\sigma u$ plus $Ch^2\sigma^{-2}\|u\|^2\|$.

Similarly we deal $\operatorname{Re}(Lu, u) = \operatorname{Re}(L\psi_\sigma u, \psi_\sigma u) + \operatorname{Re}(L\psi'_\sigma u, \psi'_\sigma u)$ and the absolute value of the second term does not exceed $m(1 - a^2)^{\frac{1}{2}} T\|B_m^{1/m}\psi'_\sigma\|^2$.

We claim that

$$\operatorname{Re}(L\psi_\sigma u, \psi_\sigma u) \le C\sigma\|\psi_\sigma u\|^2 + C\sigma h^\delta; \tag{4.15}$$

we prove it later but now instead of (4.12) we arrive for $\sigma = \epsilon_0 t$ to

$$((1 - a^2) - \epsilon)P(T) \le Ch^{\delta'} + (a^m - a^2)T^{-1}\int_\gamma^T P(t)\,dt + C\gamma T^{-1}$$

with $P(t) = \|\psi_{\epsilon_0 t} u(., t)\|^2$. Then since $\nu = (a^m - a^2)/((1 - a^2) - \epsilon) < 0$ this inequality implies (4.3) again. □

Proof of (4.15). Indeed, as $h = 1$, $\|B_m^{1/m}u\| \le 1$ we from G. Grubb [5, 6] conclude that $|u(x_1)| \le Cx_1^{(m-1)/2}\|uB_m^{1/m}u\|$ and $|Lu(x_1)| \le Cx_1^{(m-1)/2}$ and therefore $|(Lu, u)| \le C\sigma^m\|B_m^{1/m}u\|^2$. Take $\sigma = 1$.

Scaling returns (4.15) as $\sigma = h$. □

Proposition 4.3. *Let $\Lambda = \Lambda_{m,X}$ be a d-dimensional operator* (1.1) *on the half-space $X = \{x \in \mathbb{R}^d, x_1 > 0\}$ with Euclidean metrics ($d \ge 2$) and $A = h\Lambda^{1/m} - 1$.*

Let $\psi \in \mathscr{C}_0^\infty([-1, 1])$, $\psi_\gamma(x) = \psi(x_1/\gamma)$, $\phi \in \mathscr{C}_0^\infty([-1, 1])$, $\varphi \in \mathscr{C}_0^\infty(\mathbb{R}^{d-1})$ supported in $\{|\xi'| \le 1 - \epsilon\}$ with $\epsilon > 0$. Finally, let $\gamma \ge h^{1-\delta}$, $T \ge Ch^{-\delta}\gamma$, $h^\delta \ge \eta \ge h^{1-\delta}T^{-1}$. Then

$$\|\phi(\eta^{-1}hD_t - 1)\varphi(hD')\psi_\gamma(x_1)e^{ih^{-1}tA}\psi_\gamma(x_1)|_{t=T}\| = O(h^s) \tag{4.16}$$

with arbitrarily large s.

Proof. By making Fourier transform $F_{x'\to h^{-1}\xi'}$ we reduce the general case to $d=1$ and operator B.

According to Proposition 4.2 $\|\phi(\eta^{-1}hD_t)\psi_\gamma e^{ih^{-1}TA}\psi\| \le h^\delta$. Thus for $s=\delta'$ (4.16) has been proven (we reduce δ' if necessary).

Without any loss of the generality we assume that $\psi(x_1)=1$ as $x_1\le 1$, $\psi(x_1)=0$ as $x_1\ge 2$. Observe that due to propagation as $t\le T$ and $x_1\ge\gamma$ we see that $\phi(\eta^{-1}hD_t)Q^+(hD_1)(1-\psi_\gamma)e^{ih^{-1}TA}\psi_\gamma$ is negligible where $Q^\pm\in\mathscr{C}^\infty(\mathbb{R})$ is supported in $\{\pm\xi_1>\epsilon\}$. Furthermore, from the standard ellipticity arguments we conclude that $\phi(\eta^{-1}hD_t)Q^0(hD_1)(1-\psi_\gamma)e^{ih^{-1}TA}\psi_\gamma$ is also negligible for $Q^0\in\mathscr{C}_0^\infty([-2\epsilon,2\epsilon])$.

Finally, due to propagation as $t\ge T$ and $x_1\ge\gamma$ we conclude that $\phi(\eta^{-1}hD_t)\psi_\gamma e^{ih^{-1}(t-T)A}Q^-(hD_1)(1-\psi_\gamma)e^{ih^{-1}TA}\psi_\gamma$ is negligible for $t\ge T$.

What is left is $\phi(\eta^{-1}hD_t)\psi_\gamma e^{ih^{-1}(t-T)A}Q^-(hD_1)\psi_\gamma e^{ih^{-1}TA}\psi_\gamma$ and since (4.16) holds for $s=\delta'$ we conclude that it holds for $s=2\delta'$ and T replaced by $2T$.

Continuing this process we see that (4.16) holds for $s=n\delta'$ and T replaced by nT. Therefore, as we redenote nT by T (and T by T/n respectively), we acquire factor $(\gamma n/T)^n$ in our estimate and it is $O(h^s)$ for any s as h is sufficiently small, $\gamma/T\le h^\delta$ and $n=s/\delta'$. □

4.2 General Case

Theorem 4.4. *Let $(\bar{x},\bar{\xi})$ be a point on the energy level 1. Consider a Hamiltonian trajectory $\Psi_t(\bar{x},\bar{\xi})$ with $\pm t\in[0,mT]$ (one sign only) with $T\ge\epsilon_0$ and assume that for each t indicated it meets ∂X transversally i.e.*

$$\text{dist}(\pi_x\Psi_t(x,\xi),\partial X)\le\epsilon \implies |\frac{d}{dt}\text{dist}(\pi_x\Psi_t(x,\xi),\partial X)|\ge\epsilon \qquad \forall t:\pm t\in[0,mT]. \tag{4.17}$$

Also assume that

$$\text{dist}(\pi_x\Psi_t(x,\xi),\partial X)\ge\epsilon_0 \qquad \text{as}\quad t=0,\ \pm t=mT. \tag{4.18}$$

Let $\epsilon>0$ be a small enough constant, Q be supported in ϵ-vicinity of (x,ξ) and $Q_1\equiv 1$ in $C_0\epsilon$-vicinity of $\Psi_t(x,\xi)$ as $t=\pm mT$. Then operator $(I-Q_1)e^{-ih^{-1}tH}Q$ is negligible as $t=\pm mT$.

Proof. (a) Obviously without any loss of the generality one can assume that there is just one reflection from ∂X (and this reflection is transversal) and that (3.1) is fulfilled in its vicinity.

Further, without any loss of the generality one can assume that Q is supported in ε-vicinity of $(\bar{x},\bar{\xi})$, $Q_1 \equiv 1$ in ε-vicinity of $\Psi_{mT}(\bar{x},\bar{\xi})$ and $T \asymp \varepsilon$ with $\varepsilon = h^{\frac{1}{2}-\delta'}$. Then both $\bar{x}$ and $\pi_x\Psi_{mT}(\bar{x},\bar{\xi})$ belong to $C_0\varepsilon$-vicinity of ∂X.

Indeed, it follows from the propagation inside of domain.

(b) Then instead of isotropic vicinities we can consider anisotropic ones: ε with respect to (x',ξ'), $h^{1-3\delta'}$ with respect to x_1 and $h^{\delta'}$ with respect to ξ_1. Let now Q and Q_1 be corresponding operators.

In this framework from the propagation inside of domain it follows that without any loss of the generality one can assume that $T \asymp \gamma = h^{1-\delta''}$ and both $\bar{x}$ and $\pi_x\Psi_{mT}(\bar{x},\bar{\xi})$ belong to $C_0\gamma$-vicinity of ∂X.

(c) Then one can employ the method of the successive approximations freezing coefficients at point $\bar{x}$ and in this case the statement of the theorem follows from the construction of Section 7.2 of [9][2)] and Proposition 4.3. We leave easy details to the reader. □

Then we arrive immediately to

Corollary 4.5. *Under standard non-periodicity condition*[3)] N_h^- *is given with* $o(h^{1-d})$*-error by the Tauberian expression with* $T = h^{1-\delta}$.

Proof. Easy details are left to the reader. □

5 Main Results

5.1 From Tauberian to Weyl Asymptotics

Now we can apply the method of successive approximations as described in Section 7.2 [2)] and prove that for operator A the Tauberian expression with

[2)] Insignificant and rather obvious modifications are required.

[3)] The set of all periodic billiards has measure zero.

$T = h^{1-\delta}$ (with sufficiently small $\delta > 0$) equals to Weyl expression $\mathsf{N}_h^{\mathsf{W}}$ with $O(h^{2-d-\delta''})$ error,

$$\mathsf{N}_h^{\mathsf{W}} = \kappa_0 h^{-d} + \kappa_{1,m} h^{1-d} + o(h^{1-m}) \tag{5.1}$$

with the standard coefficient $\kappa_0 = (2\pi)^{-d}\varpi_d \operatorname{vol}_d(X)$ and with

$$\kappa_{1,m} = (2\pi)^{1-d}\varpi_{d-1}\varkappa_m \operatorname{vol}_{d-1}(\partial X), \tag{5.2}$$

where

$$\varkappa_m = \\ = \frac{d-1}{m}\iint_1^\infty \lambda^{-(d-1)/m-1}\Bigl(\boldsymbol{e}_m(x_1,x_1,\lambda) - \pi^{-1}(\lambda-1)^{1/m}\Bigr)\,dx_1 d\lambda \tag{5.3}$$

with $\boldsymbol{e}_m(x_1,y_1,\tau) = \boldsymbol{e}_{m,1,1}(x_1,y_1,\tau)$ the Schwartz kernel of the spectral projector of operator $\boldsymbol{a}_m \coloneqq B_{m,1,1}$ introduced by (4.1):

$$\boldsymbol{a}_m = ((D_x^2+1)^{m/2})_{\mathfrak{D}} \tag{5.4}$$

Recall that vol_d and vol_{d-1} are Riemannian volumes corresponding to metrics g and its restriction to ∂X respectively and $\pi^{-1}(\lambda-1)^{1/m}$ is a Weyl approximation to $\boldsymbol{e}_{m,1}(x_1,x_1,\lambda)$. Thus we arrive to

Theorem 5.1. *Under standard non-periodicity condition the following asymptotics holds:*

$$\mathsf{N}(\tau) = \kappa_0\tau^{\frac{d}{m}} + \kappa_{1,m}\tau^{\frac{d-1}{m}} + o(\tau^{\frac{d-1}{m}}) \qquad \textit{as}\ \ \tau\to+\infty. \tag{5.5}$$

Proof. First we establish as described above asymptotics

$$\mathsf{N}_h^- = \kappa_0 h^{-d} + \kappa_{1,m}h^{1-d} + o(h^{1-d}) \qquad \text{as}\ \ h\to+0, \tag{5.6}$$

which immediately implies (5.5). □

Remark 5.2. Based on our analysis one can prove easily also the asymptotics for the Riesz means:

$$\Bigl(\mathsf{N}(\tau) - \sum_{k<r+1}\kappa_{k,m}\tau^{\frac{d-k}{m}}\Bigr) * \tau_+^{r-1} = O(\tau^{\frac{d-1}{m}}) \qquad \text{as}\ \ \tau\to+\infty, \tag{5.7}$$

and under standard non-periodicity condition

$$\Bigl(\mathsf{N}(\tau) - \sum_{k\le r+1}\kappa_{k,m}\tau^{\frac{d-k}{m}}\Bigr) * \tau_+^{r-1} = o(\tau^{\frac{d-1}{m}}) \qquad \text{as}\ \ \tau\to+\infty, \tag{5.8}$$

with some coefficients $\kappa_{k,m}$.

5.2 Discussion

The following problems seem to be challenging

Problem 5.3. As $m_1 > 0$, $m_2 > 0$ consider

$$K = K_{m_1,m_2,X} \coloneqq \Lambda_{m,X} - \Lambda_{m_1,X}\Lambda_{m_2,X} \tag{5.9}$$

on $\mathfrak{D}(\Lambda_m)$ with $m = m_1 + m_2$. From Corollary A.2 we conclude that this is a non-negative operator. Furthermore, due to [12, 13] it is a positive operator. Obviously singularities of its Schwartz kernel $K(x, y)$ belong to $\partial X \times \partial X$.

(i) Provide an effective estimate for this operator from below.

(ii) Prove that as $X = \{x \in \mathbb{R}^d : x_1 > 0\}$ with Euclidean metrics its Schwartz kernel $K(x, y) = k(x_1, y_1, x' - y')$ which is positive homogeneous of degree $-m - d$ satisfies

$$|D_x^\alpha D_y^\beta K(x, y)| \\ \le C_{\alpha\beta} x_1^{-\frac{m}{2}-\alpha_1} y_1^{-\frac{m}{2}-\beta_1} (x_1 + y_1 + |z|)^{-d-|\alpha'|+|\beta'|}. \tag{5.10}$$

(iii) In the general case in the local coordinates in which $X = \{x : x_1 > 0\}$ and $x_1 = \mathsf{dist}(x, \partial X)$ not only (5.10) holds but also

$$|D_x^\alpha D_y^\beta (K(x, y) - K^0(x, y))| \\ \le C_{\alpha\beta} (x_1 + y_1)^{-m-\alpha_1-\beta_1} (x_1 + y_1 + |z|)^{-d-|\alpha'|+|\beta'|+1} \tag{5.11}$$

where $K^0(x, y) = k(x_1, y_1, x' - y')$ and $g^{jk} = \delta_{jk}$ at point $(0, \frac{1}{2}(x' + y'))$.

Problem 5.4. For $m > 0$, $n > 0$ consider operator

$$K = K_{m,n,X} \coloneqq \Lambda_{m,X} - \Lambda_{n,X}^{m/n} \tag{5.12}$$

on $\mathfrak{D}(\Lambda_k)$ with $k = \max(m, n)$. Then this is a non-negative (non-positive) operator as $m > n$ ($m < n$ respectively. Furthermore, due to [12, 13] it is a positive (negative) operator respectively.

(i) Provide an effective estimate for this operator from below.

(ii) Prove that if $X = \{x \in \mathbb{R}^d : x_1 > 0\}$ with Euclidean metrics its Schwartz kernel $K(x,y) = k(x_1, y_1, x' - y')$ which is positive homogeneous of degree $-(m+d)$ and satisfies (5.10).

(iii) Prove that in the framework of Problem 5.3(iii) both (5.10) and (5.11) hold.

Problem 5.5. (i) Consider operators $(\Delta^{m/2})_{\mathfrak{D}}$ with $m < 0$ and the asymptotics of eigenvalues tending to $+0$.

(ii) Consider operators with degenerations like $A_{m,X} = h^m \Lambda_{m,X} + V(x)$.

(iii) Consider more general operators where instead of Δ general elliptic (matrix) operator is used.

Problem 5.6. (i) Consider Neumann boundary conditions: having smooth metrics g in the vicinity of $\bar{X}$ for each point $x \notin X$ in the vicinity of ∂X we can assign a mirror point $j(x) \in \bar{X}$ such that x and $j(x)$ are connected by a (short) geodesics orthogonal to Y at the point of intersection. Each u defined in X we can continue to the vicinity of $\bar{X}$ as $Ju(x) = \psi(x)u(j(x))$ with ψ supported in the vicinity of $\bar{X}$ and $\psi = 1$ in the smaller vicinity of $\bar{X}$. Then $\Lambda_m u = R_X \Delta^{m/2} J u$.

- Establish eigenvalue asymptotics for this operator.
- Surely we need to prove that the choice neither of metrics outside of X nor ψ is important.

(ii) One can also try $Ju(x) = -\psi(x)u(j(x))$ and prove that eigenvalue asymptotics for this operator do not differ from what we got just for continuation by 0.

Problem 5.7. Consider manifolds with all geodesic billiards closed as in Section 8.3 of [9]. To do this we need to calculate the "phase shift" at the transversal reflection point itself seems to be an extremely challenging problem.

6 Global Theory

Let us discuss fractional Laplacians defined by (1.1) in domain $X \subset \mathbb{R}^d$. Then under additional condition

$$\mathsf{dist}(x,y) \le C_0 |x-y| \qquad \forall x,y \in X \tag{6.1}$$

(where $\mathsf{dist}(x, y)$ is a "connected" distance between x and y) everything seems to work. We leave to the reader:

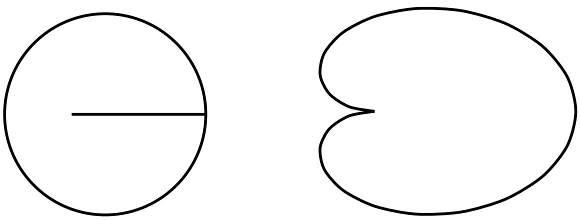
Problem 6.1. Under assumption (6.1)

(i) prove Lieb-Cwikel-Rozeblioum estimate (9.A.11) of [9].

(ii) Restore results of Chapter 9 of [9].

(iii) Reconsider examples of Sections 11.2 and 11.3 of [9].

Remark 6.2. Obviously domains with cuts and inner spikes (inner angles of 2π) do not fit (6.1). On the other hand, in the case of the domain with the cut due to non-locality of Δ^r with $r \in \mathbb{R}^+ \setminus \mathbb{Z}$ both sides of the cut "interact" and at least coefficient in the second term of two-term asymptotics may be wrong; in the case of the inner spike some milder effects are expected.



(a) (b)

Figure 1: Domain with a cut (a) and an inner spike (b).

The following problem seems to be very challenging:

Problem 6.3. (i) Investigate fractional Laplacians in domains with cuts and inner spikes and save whatever is possible.

(ii) Generalize these results to higher dimensions.

A Variational Estimates for Fractional Laplacian

A.1 Variational Estimates for Fractional Laplacian

We follow here R. Frank and L. Geisinger [4]. This is Lemma 19 and the next paragraph of their paper:

Lemma A.1. *(i) Let B be a non-negative operator with* $\operatorname{Ker} B = \{0\}$ *and let P be an orthogonal projection. Then for any operator monotone function $\phi : (0, \infty) \to \mathbb{R}$,*

$$P\phi(PBP)P \geq P\phi(B)P. \tag{A.1}$$

(ii) If, in addition, B is positive definite and ϕ is not affine linear, then $\phi(PBP) = P\phi(B)P$ implies that the range of P is a reducing subspace of B.

We recall that, by definition, the range of P is a reducing subspace of a non-negative (possibly unbounded) operator if $(B + \tau)^{-1} \operatorname{Ran} P \subset \operatorname{Ran} P$ for some $\tau > 0$. We note that this is equivalent to $(B + \tau)^{-1}$ commuting with P, and we see that the definition is independent of τ since

$$\begin{aligned}
&(B + \tau')^{-1} P - P(B + \tau')^{-1} \\
&\quad = (B + \tau)(B + \tau')^{-1} \left((B + \tau)^{-1} P - P(B + \tau)^{-1} \right) (B + \tau)(B + \tau')^{-1}.
\end{aligned}$$

We refer to the proof given there.

Corollary A.2. *The following inequality holds*

$$\Lambda_{m,X} \leq \Lambda_{n,X}^{m/n} \qquad \text{as} \ \ 0 < m < n. \tag{A.2}$$

Proof. Plugging into (A.1) $B = \Delta^{n/2}$ in $\mathbb{R}^d$, $P = \theta_X(x)$ and $\phi(\lambda) = \lambda^{m/n}$ we get (A.2). □

Repeating arguments of Proposition 20 and following it Subsection 6.4 of R. Frank and L. Geisinger [4] (powers of operators will be different but also negative) we conclude that

Proposition A.3. *Let $d \geq 2$. Then $-\varkappa_m$ is positive strictly monotone increasing function of $m > 0$.*

We leave details to the reader.

A.2 μ-Transmission Property

Proposition 1 of G. Grubb [6] claims that

Proposition A.4. *A necessary and sufficient condition in order that $R_X Pu \in \mathscr{C}^\infty(\bar{X})$ for all $u \in \mathscr{E}_\mu(\bar{X})$ is that P satisfies the μ-*transmission condition *(in short: is of type μ), namely that*

$$\partial_x^\beta \partial_\xi^\alpha p_j(x, -N) = e^{\pi i(m-2\mu-j-|\alpha|)} \partial_x^\beta \partial_\xi^\alpha p_j(x, N) \qquad \forall x \in \partial\Omega, \tag{A.3}$$

for all j, α, β, where N denotes the interior normal to ∂X at x, m is an order of classical pseudo-differential operator P and for $\mu \in \mathbb{C}$ with $\operatorname{Re}\mu > -1$.

Here $\mathscr{E}_\mu(\bar{X})$ denotes the space of functions u such that $u = E_X d(x)^\mu v$ with $v \in \mathscr{C}^\infty(\bar{X})$ where E_X is an operator of extension by 0 to $\mathbb{R}^d \setminus X$ and $d(x) = \operatorname{dist}(x, \partial X)$.

Observe that for $\mu = 0$ we have an ordinary transmission property (see Definition 1.4.3) of [9].

Comments

This project started when I learned to my surprise that fractional Laplacians are of the interest to probability theory: which seem to be of interest to probability theory starting from R. M. Blumenthal, R. M. and R. K. Getoor [3] and then by R. Bañuelos and T. Kulczycki [1], R. Bañuelos, T. Kulczycki and B. Siudeja [2], M. Kwaśnicki [11]; some of these authors were interested in "Ivrii-type results" (i.e. generalizations from $m = 2$ to $m \in (0, 2)$

Those operators were formulated in the framework of stochastic processes and thus were not accessible for me until I found paper R. Frank and L. Geisinger [4] provided definition we follow here. They showed that the trace has a two-term expansion regardless of dynamical assumptions[4)], and the second term in their expansion paper [4] defined by (3.2)–(3.3) is closely related to $\kappa_{1,m}$. It corresponds to $r = 1$ in Remark 5.2.

Furthermore, I learned that one-term asymptotics for more general operators (albeit without remainder estimate) was obtained by G. Grubb [7].

[4)] The fact that R. Frank and L. Geisinger obtain a second term regardless of dynamical assumptions is simply due to the fact that they study $\operatorname{Tr}(f(\Lambda_{m,X}))$ with $f(\lambda) = -\lambda\theta(-\lambda)$, which is one order smoother than $f(\lambda) = \theta(-\lambda)$.

Very recently I used the ideas of Section 4 to study sharp spectral asymptotics for Dirichlet-to-Neumann operator in [10].

I express my gratitudes to G. Grubb and R. Frank for pointing to rather nasty errors in the previous version of this article and very useful comments, and to R. Bañuelos for very useful comments. I also express my gratitudes to the referee of this paper for several useful remarks.

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Spectral Asymptotics for Dirichlet to Neumann Operator in the Domains with Edges*,†

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Abstract

We consider eigenvalues of the Dirichlet-to-Neumann operator for Laplacian in the domain (or manifold) with edges and establish the asymptotics of the eigenvalue counting function

$$\mathsf{N}(\lambda)=\kappa_0\lambda^d+O(\lambda^{d-1})\qquad \text{as}\ \ \lambda\to+\infty,$$

where d is dimension of the boundary. Further, in certain cases we establish two-term asymptotics

$$\mathsf{N}(\lambda)=\kappa_0\lambda^d+\kappa_1\lambda^{d-1}+o(\lambda^{d-1})\qquad \text{as}\ \ \lambda\to+\infty.$$

We also establish improved asymptotics for Riesz means.

1 Introduction

Let X be a compact connected $(d+1)$-dimensional Riemannian manifold with the boundary Y, regular enough to properly define operators J and Λ below[1)]. Consider *Steklov problem*

$$\Delta w=0 \qquad \text{in}\ \ X, \tag{1.1}$$

$$(\partial_\nu+\lambda)w|_Y=0, \tag{1.2}$$

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1) Manifolds with edges are of this type.

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where Δ is the positive Laplace-Beltrami operator[2)], acting on functions on X, and ν is the unit inner normal to Y. In the other words, we consider eigenvalues of the Dirichlet-to-Neumann operator. For v, which is a restriction to Y of $\mathscr{C}^2$ function, we define $Jv = w$, where $\Delta w = 0$ in X, $w|_Y = v$, and $\Lambda v = -\partial_\nu Jv|_Y$.

Definition 1.1. Λ is called *Dirichlet-to-Neumann operator*.

The purpose of this paper is to consider manifold with the boundary which has edges: i.e. each point $y \in Y$ has a neighbourhood U in $\bar{X} := X \cap Y$, which is the diffeomorphic either to $\mathbb{R}^+ \times \mathbb{R}^d$ (then y is a *regular point*), or to $\mathbb{R}^{+2} \times \mathbb{R}^{d-1}$ (then y is an *inner edge point*) or to $(\mathbb{R}^2 \setminus \mathbb{R}^{-2}) \times \mathbb{R}^{d-1}$ (then y is an *outer edge point*). Let Z_{inn} and Z_{out} be sets of the inner and outer edge points respectively, and $Z = Z_{\mathsf{inn}} \cup Z_{\mathsf{out}}$.

One can prove easily the following proposition:

Proposition 1.2. *(i)* Λ *is a non-negative essentially self-adjoint operator in* $\mathscr{L}^2(Y)$*;* $\operatorname{Ker}(\Lambda)$ *consists of constant functions.*

(ii) Λ *has a discrete accumulating to infinity spectrum with eigenvalues* $0 = \lambda_0 < \lambda_1 \le \ldots$ *could be obtained recurrently from the following variational problem:*

$$\int_X |\nabla w|^2\, dx \mapsto \min(= \lambda_n) \tag{1.3}$$

$$\text{as} \quad \int_Y |w|^2\, dx' = 1, \qquad \int_Y w w_k^\dagger\, dx' = 0 \quad \text{for} \quad k = 0, \ldots, n-1.$$

Corollary 1.3. *The number of eigenvalues of* Λ*, which are less than* λ*, equals to the maximal dimension of the linear space of* $\mathscr{C}^2$*-functions, on which the quadratic form*

$$\int_X |\nabla w|^2\, dx - \lambda \int_Y |w|^2\, dx' \tag{1.4}$$

is negative definite.

Proposition 1.4. *Operator* Λ *has a domain* $\mathscr{H}^1(Y)$ *and*

$$\|\Lambda u\|_Y + \|u\|_Y \asymp \|u\|_{\mathscr{H}^1(Y)}, \tag{1.5}$$

where $(.,.)$ *and* $\|.\|$ *denote* $\mathscr{L}^2$ *inner product and norm.*

[2)] Defined via quadratic forms.

Proof. Let $L = \ell\cdot\nabla$, ℓ be a vector field which makes an acute angle with the inner normal (at Z–with both inner normals). Consider

$$0 = -(\Delta w, Lw)_X = (\nabla w, \nabla Lw)_X + (\partial_\nu w, Lw)_Y = \int Q(\nabla w)\,dy + O(\|w\|^2_{\mathscr{H}^1(X)}), \tag{1.6}$$

where

$$Q(\nabla w) = (\nu\cdot\nabla w)(\ell\cdot\nabla w) - \frac{1}{2}\nu\cdot\ell|\nabla w|^2. \tag{1.7}$$

This quadratic form has one positive and d negative eigenvalues. Further, on the subspace orthogonal to ℓ, all eigenvalues are negative. Then

$$\|\partial_\nu w\|^2 + C\|w\|^2_{\mathscr{H}^1(X)} \asymp \|w\|^2_{\mathscr{H}(Y)}. \tag{1.8}$$

Combined with the estimate for $\|w\|^2_{\mathscr{H}^1(X)} \le C\|w\|^2_{\mathscr{H}^{\frac{1}{2}}(Y)}$ it implies the statement. □

Remark 1.5. (i) If Y is infinitely smooth, then Λ is the first-order pseudodifferential operator on Y with the principal symbol $(g_Y(x,\xi))^{1/2}$, where g_Y is the restriction of the metrics to Y. Then the standard results hold:

$$\mathsf{N}(\lambda) = \kappa_0\lambda^d + O(\lambda^{d-1}) \qquad \text{as}\ \ \lambda\to+\infty \tag{1.9}$$

with the standard coefficient $\kappa_0 = (2\pi)^{-d}\omega_d\,\mathsf{mes}(Y)$, where $\mathsf{mes}(Y)$ means d-dimensional volume of Y, ω_d is the volume of the unit ball in $\mathbb{R}^d$. We also can get two-term asymptotics with the same remainder estimate for $\mathsf{N}(\lambda)*\lambda_+^{r-1}$, $0<r\le 1$.

(ii) Moreover, if the set of all periodic geodesics of Y has measure 0, then

$$\mathsf{N}(\lambda) = \kappa_0\lambda^d + \kappa_1\lambda^{d-1} + o(\lambda^{d-1}) \qquad \text{as}\ \ \lambda\to\infty. \tag{1.10}$$

We also can get two-term asymptotics (three-term for $r=1$) with the same remainder estimate for $\mathsf{N}(\lambda)*\lambda_+^{r-1}$, $0<r\le 1$. The same asymptotics, albeit with a larger number of terms, hold for $r>1$.

(iii) "Regular" singularities of the dimension $<(d-1)$ (like conical points in $3\mathsf{D}$) do not cause any problems for asymptotics of $\mathsf{N}(\lambda)$—we can use a rescaling technique to cover them; moreover, in the framework of this paper they would not matter even combined with edges (like vertices in $3\mathsf{D}$).

2 Dirichlet-to-Neumann Operator

2.1 Toy-Model: Dihedral Angle

Let $Z=\mathbb{R}^{d-1}$ with the Euclidean metrics, $X=\mathcal{X}\times Z$, $Y=\mathcal{Y}\times Z$, where $\mathcal{X}$ is a planar angle of solution α, $0<\alpha\le 2\pi$, $\mathcal{Y}=\mathcal{Y}_1\cup\mathcal{Y}_2$, $\mathcal{Y}_j$ are rays (see Figure 2).

Then one can identify Y with $\mathbb{R}^d$ with coordinates (s,z), where $z\in Z$ and

- $s=\mathsf{dist}(y,Z)$ for for a point $y\in Y_1=\mathcal{Y}_1\times Z$,

- $s=-\mathsf{dist}(y,Z)$ for for a point $y\in Y_2=\mathcal{Y}_2\times Z$.

Then we have a Euclidean metrics and a corresponding positive Laplacian Δ_Y on Y.

Remark 2.1. (i) We can consider any angle $\alpha>0$, including $\alpha>2\pi$ (in which case X could be defined in the polar coordinates, but then we need to address some issues with the domain of operator).

(ii) If $\alpha=\pi$, then $\Lambda=\Delta_Y^{1/2}$.

(iii) We say that X is a *proper angle* if $\alpha\in(0,\pi)$ and that X is a *improper angle* if $\alpha\in(\pi,2\pi)$. We are not very concerned about $\alpha=\pi$, 2π since these cases will be forbidden in the general case.

For this toy-model we can make a partial Fourier transform $F_{z\to\zeta}$ and then study equation in the planar angle:

$$\Delta_2 w+w=0, \tag{2.1}$$

where Δ_2 is a positive 2D-Laplacian and we made also a change of variables $x''\mapsto|\zeta|\cdot x''$, $x''=(x_1,x_2)$. Denote by $\bar{J}$ and $\bar{\Lambda}$ operators J and Λ for (2.1). This problem is extensively studied in Appendix A.1.

Then we can use the separation of variables. Singularities at the vertex for solutions to (2.1) and $w|_Y=0$, are the same as for $\Delta_2 w=0$, $w|_Y=0$ and they are combinations of $r^{\pi n/\alpha}\sin(\pi n\theta/\alpha)$ with $n=1,2,...$, where $(r,\theta)\in\mathbb{R}^+\times(0,\alpha)$ are polar coordinates.

This show the role of α: if $\alpha\in(0,\pi)$ those functions are in $\mathscr{H}^{\sigma}_{\mathsf{loc}}(\mathcal{X})$ with $\sigma<1+\pi n/\alpha$, and $\partial_\nu w|_Y$ belong to $\mathscr{H}^{\sigma-3/2}_{\mathsf{loc}}(\mathcal{Y})$.

One can prove easily the following Propositions 2.2 and 2.3 below:

Proposition 2.2. *The following are bounded operators*

$$\Delta_{\mathsf{D}}^{-1} : \mathscr{H}^{\sigma}(X) \to \mathscr{H}^{\sigma+2}(X), \tag{2.2}$$

$$J : \mathscr{H}^{\sigma+\frac{3}{2}}(Y) \to \mathscr{H}^{\sigma+2}(X), \tag{2.3}$$

$$\Lambda : \mathscr{H}^{\sigma+\frac{3}{2}}(Y) \to \mathscr{H}^{\sigma+\frac{1}{2}}(X), \tag{2.4}$$

where Δ_{D} *is an operator* Δ *with zero Dirichlet boundary conditions on* Y *and*

- $\sigma \in [-\frac{1}{2}, 0]$, *if* $\alpha \in (0, \pi)$, *and*

- $\sigma \in [-\frac{1}{2}, \bar{\sigma})$ *with* $\bar{\sigma} = \pi/\alpha - 1$ *otherwise.*

Proposition 2.3. *For equation* (2.1) *in* $\mathcal{X}$

$$\bar{\Lambda} - (D_s^2 + 1)^{1/2} = \sum_{j+k\le 1} D_s^j \bar{K}_{jk} D_s^k\,, \tag{2.5}$$

where operators $\bar{K}_{jk}$ *have Schwartz kernels* $\bar{K}_{jk}(s, s')$ *such that*

$$|D_s^p D_{s'}^q \bar{K}_{jk}(s, t')| \le \\ C_{pqm} |s|^{-(\bar{\sigma}-p)_-} |s'|^{-(\bar{\sigma}-q)_-} (|s| + |s'|)^{-p-q+(\bar{\sigma}-p)_- + (\bar{\sigma}-q)_-} (|s| + |s'| + 1)^m \tag{2.6}$$

and $l_\pm := \max(\pm l, 0)$ *and* m *is arbitrarily large.*

Then

Corollary 2.4. *For the toy-model in* X

$$\Lambda - \Delta_Y^{1/2} = \sum_{j+k\le 1} D_s^j K_{jk} D_s^k\,, \tag{2.7}$$

where operators K_{jk} *have Schwartz kernels*

$$K_{j,k}(x', s; y', s') = (2\pi)^{1-d} \iint |\xi'|^{2-j-k} \bar{K}_{jk}(s|\xi'|,\, s'|\xi'|) e^{-i\langle x'-y', \xi'\rangle}\, d\xi'. \tag{2.8}$$

2.2 General Case

Consider now the general case. In this case we can again introduce coordinate s on Y and consider Y as a Riemannian manifold, but with the metrics which is only $\mathscr{C}^{0,1}$ (Lipschitz class); more precisely, it is $\mathscr{C}^\infty$ on both Y_1 and Y_2, but the first derivative with respect to s may have a jump on Z. It does not, however, prevent us from introduction of Δ_Y and therefore $\Delta_Y^{\frac{1}{2}}$, but the latter would not be necessarily the classical pseudodifferential operator.

We want to exclude the degenerate cases of the angles π and 2π. So, let us assume that

(2.9) $Z = \{x\colon x_1 = x_2 = 0\}$ and $X = Z \times \mathcal{X}$ with a planar angle $\mathcal{X} \ni (x_1, x_2)$, disjoint from half-plane and the plane with a cut.

Definition 2.5. For $z \in Z$ let $\alpha(z)$ be an internal angle between two leaves of Y at point z (calculated in the corresponding metrics). Due to our assumption either $\alpha(z) \in (0, \pi)$ or $\alpha(z) \in (\pi, 2\pi)$. Let Z_j be a connected component of Z.

(i) Z_j is a *inner edge* if $\alpha(z) \in (0, \pi)$ on Z_j, and

(ii) Z_j is an *outer edge* if $\alpha(z) \in (\pi, 2\pi)$ on Z_j.

One can prove easily

Proposition 2.6. *The following are bounded operators*

$$\Delta_{\mathsf{D}}^{-1} : \mathscr{H}^\sigma(X) \to \mathscr{H}^{\sigma+2}(X), \tag{2.10}$$

$$J : \mathscr{H}^{\sigma+\frac{3}{2}}(Y) \to \mathscr{H}^{\sigma+2}(X), \tag{2.11}$$

$$\Lambda : \mathscr{H}^{\sigma+\frac{3}{2}}(Y) \to \mathscr{H}^{\sigma+\frac{1}{2}}(X), \tag{2.12}$$

where Δ_{D} is an operator Δ with zero Dirichlet boundary conditions on Y and

(i) $\sigma \in [-\frac{1}{2}, 0]$, if $\alpha(z) \in (0, \pi)$ $\forall z \in Z$, and

(ii) $\sigma \in [-\frac{1}{2}, \bar{\sigma})$ with $\bar{\sigma} = \pi/\bar{\alpha} - 1$, $\bar{\alpha} = \max_{z \in Z} \alpha(z)$ otherwise.

One can also prove easily

Proposition 2.7. *In the general case, assuming that* $Z = \{x\colon x_1 = x_2 = 0\}$ *and* $X = Z \times \mathcal{X}$ *with a planar angle* $\mathcal{X} \ni (x_1, x_2)$ *of solution* $\in (0,\pi)\cup(\pi,2\pi)$

$$\Lambda - \Delta_Y^{1/2} = b + \sum_{j+k\le 1} D_s^j K_{jk} D_s^k\,, \tag{2.13}$$

where b *is a bounded operator and operators* K_{jk} *have Schwartz kernels and*

$$K_{j,k}(x',s;y',s') = (2\pi)^{1-d}\iint |\xi'|^{2-j-k}\bar{K}_{jk}\bigl(\frac{1}{2}(x'+y'), s|\xi'|,\, s'|\xi'|\bigr)\, e^{-i\langle x'-y',\xi'\rangle}\,d\xi'. \tag{2.14}$$

Remark 2.8. On the distances $\gtrsim 1$ from Z, b is a classical 0-order pseudodifferential operator, on the distance $\gtrsim |\xi'|^{-1+\delta}$ it is a rough 0-order pseudodifferential operator[3)].

3 Microlocal Analysis

3.1 Propagation of Singularities near Edge

We are going to consider microlocal analysis near point $(\bar{x},\bar{\xi}'')\in T^*Z$ under assumption (2.9). In our approach we use definition of operator Λ rather than its description of the previous Section 2. So, let $x=(x'';x')\in\mathbb{R}^2\times\mathbb{R}^{d-1}$.

Proposition 3.1. *(i) Let* $q_j = q_j(\xi')$ *(*$j=1,2$*) be two symbols, constant as* $|\xi'|\ge C$*. Assume that the* $\operatorname{dist}(\operatorname{supp}(q_1),\operatorname{supp}(q_2))\ge\epsilon$*.*

Consider h*-pseudodifferential operators* $Q_j = q_j^{\mathrm{w}}(h^{-1}D')$*,* $j=1,2$*. Then the operator norms of*

$$(3.1)_{1,2}\qquad Q_1\Delta_{\mathrm{D}}^{-1}Q_2:\mathscr{L}^2(X)\to\mathscr{H}^2(X),\qquad Q_1JQ_2:\mathscr{H}^{\frac{1}{2}}(Y)\to\mathscr{H}^2(X),$$

$$(3.1)_3\qquad Q_1\Lambda Q_2:\mathscr{H}^1(Y)\to\mathscr{L}^2(Y)$$

do not exceed $C'h^s$ *with arbitrarily large* s *where* Δ_{D} *is an operator* Δ *with zero Dirichlet boundary conditions on* Y*.*

(ii) Let $Q_j(x')$ *(*$j=1,2$*) be two functions. Then operators* $(3.1)_{1-3}$ *are infinitely smoothing by* x'*.*

---

3) I. e. with the symbols such that $|D_x^\alpha D_\xi^\beta|\le C_{\alpha\beta}\rho^{-|\beta|}\gamma^{-|\alpha}$ with $\rho\gamma\ge h^{1-\delta}$, $\rho\gamma\ge h^{1-\delta}$. Here $\rho=1$, $\gamma=|x|$.

Proof. (i) Without any loss of the generality one can assume that q_j are constant also in the vicinity of 0. Then the operator norms of $[Q_j, \Delta]\Delta_{\mathsf{D}}^{-1}$ in $\mathscr{L}^2(X)$ do not exceed Ch; replacing Q_j by $Q_j^{(n)}$ with $Q_j^{(0)} = Q_j$ and $Q_j^{(n)} := [Q_j^{(n-1)}, \Delta]\Delta_{\mathsf{D}}^{-1}$ for $j = 1, 2, ...$, we prove by induction that the operator norms of $Q_j^{(n)}$ in in $\mathscr{L}^2(X)$ do not exceed Ch^n. Then one can prove by induction easily that the operator norm of $(3.1)_1$ does not exceed Ch^s.

Then one can prove easily that the operator norm of $(3.1)_{2,3}$ do not exceed Ch^s as well. It concludes the proof of Statement (i).

(ii) Statement (ii) is proven by the same way. □

Let $u(x, y, t)$ be Schwartz kernel of $e^{it\Lambda}$, $x, y \in Y$.

Proposition 3.2. *Consider h-pseudodifferential operator $Q = q^{\mathsf{w}}(x', h^{-1}D')$ where q vanishes $\{|\xi'| \le c_0\}$. Let $\chi \in \mathscr{C}_0^\infty(\mathbb{R})$, $T \ge h^{1-\delta}$. Then operator norms of $F_{t\to\tau}\chi_T(t)Q_x u$ and $F_{t\to\tau}\chi_T(t)u\,{}^tQ_y$ do not exceed $C'_T h^s$ for $\tau \le c$ for $c_0 = c_0(c)$.*

Proof. One need to consider $v = e^{it\Lambda}f$, $f \in \mathscr{H}^1(Y)$, $\|f\|_{\mathscr{L}^2(Y)} = 1$ and observe that it satisfies $(D_t - \Lambda)v = 0$. Using (1.5) we see that operator $(D_t - V)$ is elliptic in $\{|\xi'| \ge c_0, \tau \le c\}$ while Proposition 3.1 ensures its locality. □

Therefore, in what follows

Remark 3.3. Studying energy levels $\tau \le c$ we can always apply cut-out domain $\{|\xi'| \ge c_0\}$.

Now we can study the propagation of singularities. Let us prove that the propagation speed with respects to x and ξ' do not exceed C_0. For this and other our analysis we need the following Proposition 3.4:

Proposition 3.4. *For h-pseudodifferential operator $Q = q^{\mathsf{w}}(x, hD')$ the following formula onnecting commutators $[\Delta, Q]$ and $[\Lambda + \partial_\nu, Q]$ holds:*

$$-\operatorname{Re} i([\Delta, Q]Jv, Jv)_X = \operatorname{Re} i(([\Lambda, Q] + [\partial_\nu, Q])v, v)_Y \tag{3.2}$$

Proof. First, consider real valued symbol $q=q(x,\xi')$ and $Q=q^{\mathrm{w}}(x,hD')$ its Weyl quantization. Let v denote just any function on Y and V its continuation as a harmonic function. Then for $w=Jv$

$$\begin{aligned}0=(Q\Delta w,w)_X=(\Delta Qw,w)-([\Delta,Q]w,w)_X=\\ -([\Delta,Q]w,w)_X+(Qw,\Delta w)_X-(\partial_\nu Qw,w)_Y+(Qw,\partial_\nu w)_Y=\\ -([\Delta,Q]w,w)_X-(Q\partial_\nu w,w)_Y-([\partial_\nu,Q]w,w)_Y+(Qw,\partial_\nu w)_Y=\\ -([\Delta,Q]w,w)_X+(Q\Lambda v,v)_Y-([\partial_\nu,Q]v,v)_Y-(v,Q\Lambda v)_Y=\\ -([\Delta,Q]w,w)_X-(\Lambda Qv,v)_Y-([\partial_\nu,Q]v,v)_Y,\end{aligned}$$

which implies (3.2). □

Now we can prove that at energy levels $\tau\le c$ the propagation speed with respects to x and ξ' do not exceed $C_0=C_0(c)$.

Proposition 3.5 [4]**.** *Let* $Q_j=q_j^{\mathrm{w}}(x,hD')$ *and* $\mathsf{dist}(\mathsf{supp}(q_1),\mathsf{supp}(q_2))\ge C_0T$ *with fixed* $T>0$*. Let* $\chi\in\mathscr{C}_0^\infty([-1,1])$*. Then for* $\tau\le c$

$$|F_{t\to h^{-1}\tau}\bigl(\chi_T(t)Q_{1x}u\,{}^tQ_{2y}\bigr)|\le Ch^m,\tag{3.3}$$

where here and below m *is an arbitrarily large exponent and* $C=C_m$*.*

Proof. (i) The proof is the standard one for propagation with respect to (x',ξ'): we consider $\phi(x',\xi',t)$ and prove that under the microhyperbolicity condition

$$\phi_t-\{|\xi'|,\phi\}\ge\epsilon_0,\tag{3.4}$$

which is equivalent to

$$2\phi_t-|\xi'|^{-1}\{|\xi'|^2,\phi\}\ge 2\epsilon_0|\xi'|,\tag{3.5}$$

our standard propagation theorem (see Theorem 2.1.2) holds, just repeating arguments of its proof, using equality (3.2) and the fact that $\|Jv\|_{\mathscr{H}^{1/2}(X)}\asymp\|v\|_{\mathscr{L}^2(Y)}$.

Then we plug $\phi(x',\xi',t)=\psi(x',\xi')-t$ with $|\nabla_{x',\xi'}\psi|\le\epsilon_0$, and prove that (3.3) for $q_j=q_j(x',\xi')$.

[4] Cf. Theorem 3.1(i) of [Ivr2].

(ii) We need also prove that the propagation speed with respect to (x_1, x_2) [5] does not exceed C_0, but it is easy since for $|s| \ge \epsilon$, Λ is a first-order pseudodifferential operator with the symbol $|\xi|$. □

Remark 3.6. In fact, it follows from the proof, that the propagation speed with respect to x' do not exceed C_0, and the propagation speed with respect to ξ' does not exceed $C_0|\xi'|$ with C_0, which does not depend on restriction $\tau \le c$. Meanwhile, the propagation speed with respect (x_1, x_2) does not exceed 1.

Next we prove that at energy levels $\tau = 1$ the propagation speed with respects to x' in the vicinity of $(0, \bar{\xi}')$ with $|\bar{\xi}'| \ge \epsilon_0$ is at least $\epsilon_1 = \epsilon_1(\epsilon_0)$.

Proposition 3.7 [6]**.** *Let* $Q_j = q_j^{\mathrm{w}}(x, hD')$ *and*

$$\mathsf{dist}_{x'}(\mathsf{supp}(q_1), \mathsf{supp}(q_2)) \le \epsilon_1 T$$

with fixed $T > 0$*. Let* $\chi \in \mathscr{C}_0^\infty([-1, -\frac{1}{2}] \cup [-\frac{1}{2}, -1])$*. Then for* $|\tau - 1| \le \epsilon_0$ (3.3) *holds.*

Proof. After propagation theorem mentioned in the proof of Proposition 3.5 is proven we just plug $\phi(x', \xi'.t) = \psi(x', \xi') - \epsilon t$ with $\xi' \cdot \nabla_{x'}\psi \ge 1$. □

Corollary 3.8 [7]**.** *In the framework of Proposition 3.5 consider* $|\tau - 1| \le \epsilon$*. Then*

$$|F_{t\to h^{-1}\tau}\Gamma_x \chi_T(t) u\, {}^tQ_y| \le Ch^{1-d+m}T^{-m} \tag{3.6}$$

and

$$|F_{t\to h^{-1}\tau}\Gamma_x \bigl(\bar{\chi}_{T'}(t) - \bar{\chi}_T(t)\bigr) u\, {}^tQ_y| \le Ch^{1-d+m}T^{-m}, \tag{3.7}$$

provided $\chi \in \mathscr{C}_0^\infty([-1, -\frac{1}{2}] \cup [\frac{1}{2}, 1])$, $\bar{\chi} \in \mathscr{C}_0^\infty([-1, 1])$, $\bar{\chi} = 1$ *on* $[-\frac{1}{2}, \frac{1}{2}]$, $h \le T \le T' \le T_0$ *with small constant* T_0*.*

Proof. For small constant T (3.6) follows directly from Proposition 3.7, after one proves easily that we can insert $D_{x''}$, $D_{y''}$ to the corresponding estimate, which is easy.

For $h \le T \le T_0$ we use just rescaling like in the proof of Theorem 2.1.19. Finally, (3.7) is obtained by the summation with respect to partition of unity with respect to t. □

[5] Or, equivalently, with respect to s.

[6] Cf. Theorem 3.1(ii) of [Ivr2].

[7] Cf. Corollary 2.2(ii) of [Ivr2].

This implies immediately

Corollary 3.9. $\mathsf{N}_h(\tau)$ *and* $\mathsf{N}_h(\tau)*\tau_+^{\sigma-1}$ *are approximated by the corresponding Tauberian expressions with* $T\asymp h^{1-\delta}$ *with errors* $O(h^{1-d})$ *and* $O(h^{1-d+\sigma})$ *respectively (as* $\tau=1$ *and* $h\to+0$*).*

3.2 Reflection of Singularities from the Edge

The results of the previous subsubsection are sufficient to prove *sharp spectral asymptotics* (with the remainder estimate $O(\lambda^{d-1})$), which do not require conditions of the global nature, but insufficient to prove sharper spectral asymptotics (with the remainder estimate $o(\lambda^{d-1})$), which require conditions of the global nature.

For this more ambitious purpose we need to prove that the singularities propagate along geodesic billiards on the boundary Y, reflecting and refracting on the edge Z (so billiards will be branching), and the typical singularity (with $|\xi'|<\tau$) does not stick to Z.

To do this we will follow arguments of Subsubsection 4 of [Ivr2]. Assuming (2.9) consider operator $Q=x_1D_1+x_2D_2-i/2$, which acts along Y. As an operator in $\mathscr{L}^2(Y)$ it is self-adjoint, as an operator in $\mathscr{L}^2(X)$ it is not, but differs from a self-adjoint operator $Q=x_1D_1+x_2D_2-i$ by $i/2$, which does not affects commutators.

As a result, repeating the proof of Proposition 3.4 we arrive to

(3.8) Under assumption (2.9) equality (3.2) also holds for the operator $Q=x_1D_1+x_2D_2-i$.

To apply arguments of the proof of Propositions 4.2 and then 4.3 of [Ivr2], we need to check, if operator $i[\Lambda,Q]$ is positive definite, which in virtue of (3.2) is equivalent to the same property for the form in the left:

$$\operatorname{Re}(i[\Delta,Q]w,w)-\operatorname{Re}(i[\partial_\nu,Q]w,w)_Y\ge\epsilon\|\nabla w\|^2 \text{for}\quad w\colon \Delta=0. \tag{3.9}$$

For the toy-model $i[\Delta,Q]=2(D_1^2+D_2^2)$, $i[\partial_\nu,Q]=-\partial_\nu$, and the form on the left coincides with $\|\nabla w\|^2-2\|\nabla' w\|^2$ on w in question and therefore after Fourier transform $F_{x'\to\zeta}$ and change of variables $x_{1,2}$ it boils down to the inequality

$$\|\nabla w\|^2-\|w\|^2\ge\epsilon(\|\nabla w\|^2+\|w\|^2)\qquad \text{for}\quad w\colon \Delta_2 w+w=0 \tag{3.10}$$

for two-dimensional Δ_2, norms and scalar products.

This inequality is explored in Appendix A.1, and in virtue of Proposition A.11 (3.10) holds for $\alpha \in (\pi, 2\pi)$. Meanwhile due to Proposition A.16 (3.10) fails for $\alpha \in (0, \pi)$.

Therefore we arrive to

Proposition 3.10 [8]**.** *Consider two-dimensional toy-model (planar angle) with $\alpha \in (\pi, 2\pi)$.*

Let $\psi \in \mathscr{C}_0^\infty([-1,1])$, $\psi_\gamma(x) = \psi(x/\gamma)$ and $\phi \in \mathscr{C}_0^\infty([-1,1])$, $\tau \ge 1+\epsilon_0$. Then as $\gamma \ge h^{1-\delta}$, $T \ge C_0\gamma$, $h^\delta \ge \eta \ge h^{1-\delta}T^{-1}$

$$\|\phi(\eta^{-1}(hD_t - \tau))\psi_\gamma e^{it\Lambda}\psi_\gamma|_{t=T}\| \le CT^{-1}\gamma + Ch^{\delta'}. \tag{3.11}$$

Proof. Proof follows the proof of Proposition 4.2 of [Ivr2] with $m=1$, and uses equality (3.2) to reduce calculation of the commutator $[\Lambda, Q]$ to the calculation of the commutator $[\Delta, Q]$. □

Proposition 3.11 [9]**.** *Consider $(d+1)$-dimensional toy-model (dihedral angle) with $\alpha \in (\pi, 2\pi)$.*

Let $\psi \in \mathscr{C}_0^\infty([-1,1])$, $\psi_\gamma(x) = \psi(x_1/\gamma)$, $\phi \in \mathscr{C}_0^\infty([-1,1])$, $\varphi \in \mathscr{C}_0^\infty(\mathbb{R}^{d-1})$ supported in $\{|\xi'| \le 1-\epsilon\}$ with $\epsilon > 0$. Finally, let $\gamma \ge h^{1-\delta}$, $T \ge Ch^{-\delta}\gamma$, $h^\delta \ge \eta \ge h^{1-\delta}T^{-1}$. Then

$$\|\phi(\eta^{-1}(hD_t - 1))\varphi(hD')\psi_\gamma(x_1)e^{it\Lambda}\psi_\gamma(x_1)|_{t=T}\| = O(h^m) \tag{3.12}$$

with arbitrarily large m.

Proof. Proof follows the proof of Proposition 4.3 of [Ivr2] with $m=1$. □

Now we can consider the general case. Consider a point $\bar{z} = (\bar{x}, \bar{\xi}') \in T^*Z$, $|\bar{x}'| < 1$.

We can raise to points $\bar{z}^\pm = (\bar{x}, \bar{\xi}^\pm) \in T^*Y_{1,2}|_Z$ with $|\bar{\xi}^\pm| = 1$ and $\iota\bar{z}^\pm = \bar{z}$, where $\iota(x,\xi) = (x,\xi') \in T^*Z$ for $(x,\xi) \in T^*Y|_Z$.

Consider geodesic trajectories $\Psi_t(\bar{z}^\pm)$, going from $\bar{z}^\pm)$ into $T^*Y_{1,2}$ for $t<0$, $|t|<\epsilon$; this distinguishes these two points.

We also can consider geodesic trajectories $\Psi_t(\bar{z}^\pm)$, going from $\bar{z}^\mp$ into $T^*Y_{1,2}$ for $t>0$, $|t|<\epsilon$.

Let $\iota^{-1}\bar{z} = \{\bar{z}^+, \bar{z}^-\}$ and let $\Psi_t(\iota^{-1}\bar{z})$ be obtained as a corresponding union as well[10]. So, for such point $\bar{z}$ $\Psi_t(\iota^{-1}z)$ with $t<0$ consists of two

[8] Cf. Proposition 4.2 of [Ivr2].

[9] Cf. Proposition 4.3 of [Ivr2].

[10] So we actually restrict ι to $S^*Y|_Z$ and ι^{-1} to B^*Z.

incoming geodesic trajectories, $\Psi_t(\iota^{-1}z)$ with $t<0$ consists of two outgoing geodesic trajectories. Similarly, for $z\in (T^*(Y\setminus Z))$ we can introduce $\Psi_t(z)$: when trajectory hits Z it branches.

Theorem 3.12 [11]**.** *Consider a point $z=(x,\xi)\in T^*Y$, $|\xi|=1$. Consider a (branching) geodesic trajectory $\Psi_t(z)$ with $\pm t\in[0,T]$ (one sign only) with $T\ge\epsilon_0$ and assume that for each t indicated it meets ∂X transversally i.e.*

$$\operatorname{dist}(\pi_x\Psi_t(x,\xi),\partial X)\le\epsilon \implies |\frac{d}{dt}\operatorname{dist}(\pi_x\Psi_t(x,\xi),\partial X)|\ge\epsilon \qquad \forall t:\pm t\in[0,mT]. \tag{3.13}$$

Also assume that

$$\operatorname{dist}(\pi_x\Psi_t(x,\xi),\partial X)\ge\epsilon_0 \qquad \text{as}\quad t=0,\ \pm t=T. \tag{3.14}$$

Let $\epsilon>0$ be a small enough constant, Q be supported in ϵ-vicinity of (x,ξ) and $Q_1\equiv 1$ in $C_0\epsilon$-vicinity of $\Psi_t(x,\xi)$ as $t=\pm T$. Then operator $(I-Q_1)e^{-it\Lambda}Q$ is negligible as $t=\pm mT$.

Proof. Proof follows the proof of Theorem 4.4 of [Ivr2] with $m=1$. □

Adapting construction of the "dependence set" to our case, we arrive to the following

Definition 3.13. (i) The curve $z(t)$ in T^*Y is called a *generalized geodesic billiard* if a.e.

$$\frac{dz}{dt}\in K(z), \tag{3.15}$$

where

(a) $K(z)=\{H_g(z)\}$, $g(z)$ is a metric form, if $z\in T^*(Y\setminus Z)$,

(b) $K(z)=\{H_g(z')\colon z'\in\iota^{-1}\iota z\}$, if $z\in T^*Y|_Z$.

(ii) Let $\Psi_t(z)$ for $t\gtrless 0$ be a set of points $z'\in T^*Y$ such that there exists generalized geodesic billiard $z(t')$ with $0\lessgtr t'\lessgtr t$, such that $z(0)=z$ and $z(t)=z'$. Map $(z,t)\mapsto\Psi_t(z)$ is called a *generalized (branching) billiard flow.*

[11] Cf. Theorem 4.4 of [Ivr2].

(iii) Point $z \in T^*Y$ is *partially periodic* (with respect to Ψ) if for some $t \ne 0$ $z \in \Psi_t(z)$. Point $z \in T^*Y$ is *completely periodic* (with respect to Ψ) if for some $t \ne 0$ $\{z\} = \Psi_t(z)$

Then we arrive immediately to

Corollary 3.14. *Assume that Z consists only of only outer edges. Also assume that the set of all partially periodic points is zero.*

Then $\mathsf{N}_h(\tau)$ and $\mathsf{N}_h(\tau) * \tau_+^{r-1}$ are approximated by the corresponding Tauberian expressions with $T \asymp h^{1-\delta}$ with errors $o(h^{1-d})$ and $o(h^{1-d+r})$ respectively (as $\tau = 1$ and $h \to +0$).

Proof. Easy details are left to the reader. □

4 Main Results

4.1 From Tauberian to Weyl Asymptotics

Now we can apply the method of successive approximations as described in Section 7.2, considering an unperturbed operator

(a) As one in $\mathbb{R}^d$, with the metrics, frozen at point y, if $\mathsf{dist}(y, Z) \ge h^{1-\delta}$.

(b) As one in the dihedral edge, with the metrics, frozen at point $(y', 0)$, if $y = (y'; s)$ with $|s| = \mathsf{dist}(y, Z) \le h^{1-\delta}$,

with the following modification: We calculate Λ also this way, applying successful approximations for both Δ, when we solve $\Delta w = 0$, $w|_Y = v$, and to ∂_ν, when we calculate $\partial_\nu w|_Y$.

Then we prove that for operator $h\Lambda$ the Tauberian expression $\mathsf{N}_h^{\mathsf{T}}(1)$ for $\mathsf{N}_h^-(1)$ with $T = h^{1-\delta}$ coincides modulo $O(h^m)$ with the (generalized) Weyl expression

$$\mathsf{N}_h^{\mathsf{W}} \sim \kappa_0 h^{-d} + \kappa_1 h^{1-d} + \dots, \tag{4.1}$$

with the standard coefficient κ_0 and with $\kappa_1 = \kappa_{1,Y\setminus Z} + \kappa_{1,Z}$, where $\kappa_{1,Y\setminus Z}$ is calculated in the standard way, for the smooth boundary, and

$$\kappa_{1,Z} = (2\pi)^{1-d}\omega_{d-1}\int_Z \varkappa(\alpha(y))\, dy\,, \tag{4.2}$$

$$\varkappa(\alpha) = \int_1^\infty \int_{-\infty}^\infty \lambda^{-d}\Bigl(e_\alpha(s,s,\lambda) - \pi^{-1}(\lambda-1)\Bigr)\,dsd\lambda\,, \tag{4.3}$$

$\mathsf{e}_\alpha(s,s',\lambda)$ is a Schwartz kernel of the spectral projector of $\hat{\Lambda}$ in the planar angle of solution α and $\pi^{-1}(\lambda-1)$ is a corresponding Weyl approximation.

4.2 Main Theorems

Thus we arrive to the corresponding asymptotics for $\mathsf{N}_h^-(1)$ and from them, obviously to asymptotics for $\mathsf{N}(\tau)$:

Theorem 4.1. *Let Y be a compact manifold with edges. Then the following asymptotics hold as $\tau\to+\infty$:*

$$\mathsf{N}(\tau) = \kappa_0\tau^d + O(\tau^{d-1}) \tag{4.4}$$

and for $r>0$

$$\mathsf{N}(\tau) * \tau_+^{r-1} = \Bigl(\sum_{m<r}\kappa_m\tau^{d-r}\Bigr) * \tau_+^{r-1} + O(\tau^{d-1}). \tag{4.5}$$

Theorem 4.2. *Let Y be a compact manifold with edges. Assume that Z consists only of outer edges and that the set of all points, which are partially periodic with respect to the generalized billiard flow, has a measure 0. Then the following asymptotics hold as $\tau\to+\infty$:*

$$\mathsf{N}(\tau) = \kappa_0\tau^d + \kappa_1\tau^{d-1} + o(\tau^{d-1}) \tag{4.6}$$

and for $r>0$

$$\mathsf{N}(\tau) * \tau_+^{r-1} = \Bigl(\sum_{m\le r}\kappa_m\tau^{d-r}\Bigr) * \tau_+^{r-1} + o(\tau^{d-1}). \tag{4.7}$$

4.3 Discussion

Remark 4.3. (i) Even for standard ordinary non-branching billiards, billiard flow Ψ_t could be multivalued. However, if through point $z\in T^*(Y\setminus Z)$ (where now Y is a manifold, and Z is its boundary) passes an infinitely long in the positive (or negative) time direction billiard trajectory, which always meets Z transversally, and each finite time interval contains a finite number of reflections, then $\Psi_t(z)$ for $\pm t>0$ is single-valued. Points, which do not have such property, are called *dead-end points*. For ordinary billiards the set of dead-end points has measure zero.

(ii) For branching billiards (with velocities c_1, c_2) we can introduce the notion of the dead-end point as well: it is if at least one of the branches either meets Z non-transversally, or makes an infinite number of reflections on some finite time interval. As it was shown by Yu. Safarov and D. Vassiliev [SaVa], if c_1 and c_2 are not disjoint (our case!), the set of dead-end billiards could have positive measure.

Remark 4.4. (i) Checking non-periodicity assumption is difficult. But in some domains it will be doable. F.e. assume that $Y = Y_1 \cup Y_2$ globally is a domain of revolution, so Z is a $(d-1)$-dimensional sphere. Then the measure of the set of dead-end billiards is 0.

(ii) Assume that neither Y_1, nor Y_2 contains closed geodesics. Let $\varphi_j(\beta)$ be the length of the segment of geodesics in Y_j, with only ends on Z, where β is the reflection angle: Assume that $\varphi_j(\beta)$ are analytic and $\varphi_j(\beta) \to 0$ as

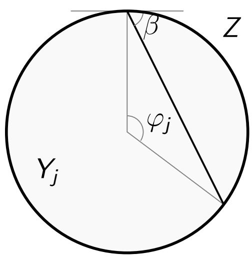


Figure 1: Trajectories on the manifold of revolution

$\beta \to +0$. Then the measure of the set of partially periodic billiards is 0.

Remark 4.5. Our arguments hold not only for compact X but also for $X \subset \mathbb{R}^{d+1}$ with the compact complement and with the metrics. stabilizing to Euclidean at infinity.

Remark 4.6. (i) In the next version of this paper we want to prove sharper asymptotics for domains with inner edges. To do this we need to understand, how singularities propagate near inner edges. One can prove that there are plenty of singularities, concentrated in $Z \times \mathbb{R} \ni (x,t)$ and $\{|\xi'| < \tau\}$. This is similar to the Rayleigh waves. And, we hope, exactly like Rayleigh waves, those singularities do not prevent us from the sharper asympotics.

What we need to prove is that the singularities in $\{|\xi'| < \tau\}$, coming from $Y \setminus Z$ transversally to Z, reflect and refract but leave Z instantly. In other words, that these two kinds of waves are completely separate. It is what I am trying to prove now.

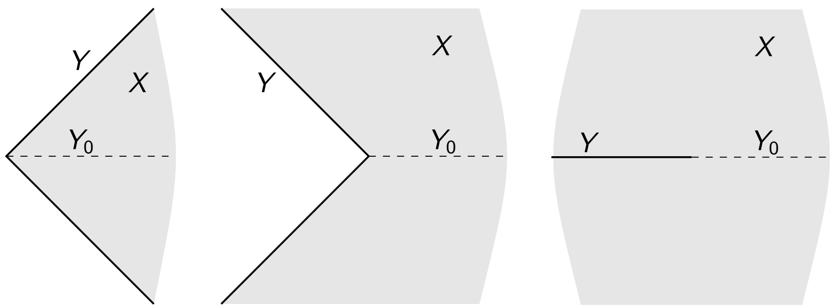
(ii) Let $\mathcal{K}$ be the linear span of the corresponding eigenfunctions. We need to prove that $\|\nabla w\| \geq \|w\|$ holds for $w = \hat{J}v$ with $v \in \mathcal{K}^{\perp}$. One can prove easily that $\|\nabla w\| = \|w\|$ for $w = \hat{J}v$ and eigenfunction v (Proposition A.16).

A Appendix

A.1 Planar Toy-Model

Preparatory Results

Here, in contrast to the whole article, $X = \{x \in \mathbb{R}^2, x_1 \geq |x_2| \cot(\alpha/2)\}$ is a planar angle of solution $\alpha \in (0, 2\pi]$ with a boundary $Y = Y_1 \cup Y_2$, $Y_{1,2} = \{x\colon x_1 = |x_2| \cot(\alpha/2),\ \pm x_2 < 0\}$ and a bisector $Y_0 = \{x\colon x_2 = 0, x_1 > 0\}$, and $\Delta = -\partial_1^2 - \partial_2^2$ is a positive Laplacian (so, for simplicity we do not write "hat").



(a) $\alpha \in (0, \pi)$ (b) $\alpha \in (\pi, 2\pi)$ (c) $\alpha = 2\pi$

Figure 2: Proper and improper angles

Remark A.1. (i) For $\alpha = \pi$ we have a regular half-plane $\{x\colon x_1 > 0\}$, and for $\alpha = 2\pi$ we have a plane with the cut $\{x\colon x_1 \leq 0,\ x_2 = 0\}$.

(ii) One can consider $\alpha > 2\pi$ on the covering of $\mathbb{R}^2$.

Consider real-valued[12] solutions of

$$Lw := (\Delta + 1)w = 0 \tag{A.1}$$

and operators J, Λ: $w = Jv$ solves (A.1) and $w|_Y = v$; $\Lambda v = -\partial_\nu w|_Y$ with $w = Jv$. Recall that ν is an inner normal to Y.

Observe that for any angle[13]

$$2\iint_X Lw \cdot w_{x_1}\, dx_1 dx_2 = \int_{\partial X} \Bigl((w_{x_1}^2 - w_{x_2}^2 - w^2)\nu_1 + 2w_{x_1}w_{x_2}\nu_2\Bigr)\, dr, \tag{A.2}$$

where dr is a Euclidean measure on Y, and the then similar formula holds with x_1 and x_2 permuted. Then for solution of (A.1)

$$\int_{\partial X} \Bigl((w_{x_1}^2 - w_{x_2}^2)(\nu_1\ell_1 - \nu_2\ell_2) + 2w_{x_1}w_{x_2}(\nu_2\ell_1 + \nu_1\ell_2) - w^2(\nu_1\ell_1 + \nu_2\ell_2)\Bigr)\, dr = 0. \tag{A.3}$$

If on $\Gamma \subset \partial X$ $\ell_1 = \nu_1$, $\ell_2 = \nu_2$, then we can calculate invariantly as if $\ell_1 = \nu_1 = 0$, $\ell_2 = \nu_2 = 1$:

$$(w_{x_1}^2 - w_{x_2}^2)(\nu_1\ell_1 - \nu_2\ell_2) + 2w_{x_1}w_{x_2}(\nu_2\ell_1 + \nu_1\ell_2) - w^2(\nu_1\ell_1 + \nu_2\ell_2) = w_\nu^2 - w_r^2 - w^2, \tag{A.4}$$

where $w_r = \partial_r w$ and $w_\nu = \partial_\nu w$.

All these formulae hold not only for the original angle, but also for the smaller angle. Then let consider as X an upper half of the symmetric angle, $\partial X = Y_2 \cup Y_0$, on Y_0 the integrand is

$$\mathcal{I} := (w_{x_2}^2 - w_{x_1}^2 - w^2)\ell_2 + 2w_{x_1}w_{x_2}\ell_1 \tag{A.5}$$

with $\ell_1 = \sin(\alpha/2)$, $\ell_2 = -\cos(\alpha/2)$.

Consider different cases:

Antisymmetric case: $w|_{Y_0} = 0$, then $\mathcal{I} = -w_{x_2}^2 \cos(\alpha/2)$ and

$$\int_{Y_2} \bigl(w_\nu^2 - w_r^2 - w^2\bigr)\, dr - \cos(\alpha/2)\int_{Y_0} w_{x_2}^2\, dx = 0. \tag{A.6}$$

Symmetric case: $w_{x_2}|_{Y_0} = 0$, then $\mathcal{I} = (w_{x_1}^2 + w^2)\cos(\alpha/2)$ and

$$\int_{Y_2} \bigl(w_\nu^2 - w_r^2 - w^2\bigr)\, dr + \cos(\alpha/2)\int_{Y_0} (w_{x_1}^2 + w^2)\, dx_1 = 0. \tag{A.7}$$

[12] For complex-valued solutions then the main inequalities with w^2 replaced by $|w|^2$ follow automatically.

[13] Not necessary symmetric with respect to x_1-axis.

Proposition A.2. *Let w satisfy* (A.1). *Let* <u>*either*</u> $\alpha \in (0, \pi]$ *and w is antisymmetric,* <u>*or*</u> $\alpha \in [\pi, 2\pi)$ *and w is symmetric. Then*

$$\|\nabla w\|^2 \ge \|w\|^2. \tag{A.8}$$

Proof. In both cases $\int_{Y_2} (|\nabla w|^2 - w^2)\, dr \ge \int_{Y_2} (w_\nu^2 - w^2)\, ds \ge 0$. Applying this inequality to the angle, shifted by t along x_1, and integrating by $t \in (0, \infty)$, we obtain a double integral (divided by $\sin(\alpha/2)$).

Moreover, one can see easily, that this inequality is strict unless $w = 0$.

Similarly, if instead of multiplying by $(\nu_1 w_{x_1} + \nu_2 w_{x_2})$ we multiply by $(x_2 w_{x_1} - x_1 w_{x_2})$, then extra terms in the double integral will be $\pm w_{x_1} w_{x_2}$ and they cancel one another. However, on Y we get $x_2 = \nu_1 r$, $x_1 = -\nu_2 r$ and therefore contribution of Y_2 will be as in above with extra factor r:

$$\int_{Y_1} \left(w_\nu^2 - w_r^2 - w^2\right) rdr. \tag{A.9}$$

On Y_0 we get extra factor $x_1 = r$, but not $\nu_2 = -\cos(\alpha/2)$, and we arrive to

Antisymmetric case: $w|_{Y_0} = 0$, then $\mathcal{I} = w_{x_2}^2 x_1$ and

$$\int_{Y_2} \left(w_\nu^2 - w_r^2 - w^2\right) rdr + \int_{Y_0} w_{x_2}^2\, x_1 dx_1 = 0. \tag{A.10}$$

Symmetric case: $w_{x_2}|_{Y_0} = 0$, then $\mathcal{I} = (-w_{x_1}^2 - w^2) x_1$ and

$$\int_{Y_2} \left(w_\nu^2 - w_r^2 - w^2\right) rdr - \int_{Y_0} (w_{x_1}^2 + w^2)\, x_1 dx_1 = 0. \tag{A.11}$$

Let us explore dependence $\Lambda = \Lambda(\alpha)$ on α. Observe first that

$$\iint \left(\nabla w \cdot \nabla w' + ww'\right) dxd_1 dx_2 = \int Lw \cdot w' - \int_{\partial X} \partial_\nu w \cdot w'\, dr \tag{A.12}$$

where (r, θ) are polar coordinates and therefore dr is an Euclidean measure on Y. It implies

$$(\Lambda v, v')_Y = \iint \left(\nabla w \cdot \nabla w' + ww'\right) dx_1 dx_2, \tag{A.13}$$

for $w = Jv$, $w' = Jv'$. Therefore

(A.14) Λ is symmetric and nonnegative operator in $\mathscr{L}^2(Y)$.

Consider $X = X(\alpha)$, $Y = Y(\alpha)$, $\Lambda = \Lambda(\alpha)$ and keep w independent on α. Let us replace α by $\alpha + \delta\alpha$ etc. Then for a symmetric X we have $\delta v = -r(\partial_\nu w)\delta\alpha = \frac{1}{2}r(\Lambda v)\delta\alpha$ and it follows from (A.13) that

$$((\delta\Lambda)v, v)_Y + 2(\Lambda v, \delta v)_Y = \frac{1}{2}\int_Y \left(|\nabla w|^2 + |w|^2\right) rdr \times \delta\alpha$$

and therefore

$$((\delta\Lambda)v, v)_Y = -\frac{1}{2}\int_Y \left(w_\nu^2 - w_r^2 - |w|^2\right) rdr \times \delta\alpha. \tag{A.15}$$

Combining with (A.10) and (A.13) we arrive to

Proposition A.3. *(i) On symmetric functions $\Lambda(\alpha)$ is monotone increasing function of α.*

(ii) On antisymmetric functions $\Lambda(\alpha)$ is monotone inreasing function of α.

Let us identify Y with $\mathbb{R} \ni s$, $s = \mp r$ on $Y_{1,2}$ respectively.

Proposition A.4. *(i) On symmetric functions $\Lambda(\pi) = (D_s^2 + I)^{\frac{1}{2}}$.*

(ii) On antisymmetric functions $\Lambda(2\pi) \geq (D_s^2 + I)^{\frac{1}{2}}$.

Proof. Statement (i) is obvious. Statement (ii) follows from the fact that on antisymmetric function v $\Lambda(2\pi)v$ coincides with $\Lambda(\pi)v^0$, restricted to $\{x_1 < 0\}$, where v^0 is v, extended by 0 to $\{x_1 > 0\}$. □

Therefore, combining Propositions A.3 and A.4 we conclude that

Corollary A.5. *(i) On symmetric functions $\Lambda(\alpha) \geq (D_s^2 + I)^{\frac{1}{2}}$ for $\alpha \in [\pi, 2\pi]$.*

(ii) On antisymmetric functions $\Lambda(\alpha) \geq (D_s^2 + I)^{\frac{1}{2}}$ for $\alpha \in (0, 2\pi]$.

Remark A.6. One can prove easily, that inequalities are strict for $\alpha \in (\pi, 2\pi]$, $\alpha \in (0, 2\pi]$ respectively.

Now we want to finish general arguments and to prove inequality (A.8) for antisymmetric w and $\alpha \in (\pi, 2\pi]$. It will be more convenient to use polar coordinates (r,θ) and notations $\mathcal{Y}_\beta = \{(r,\theta)\colon\ : \theta = \beta\}$, $\mathcal{X}_{\beta_1,\beta_2} = \{(r,\theta)\colon\ : \beta_1 \le \theta \le \beta_2\}$. Here and below $\beta_* \in [-\alpha/2, \alpha/2]$.

Recall that

$$L = -\partial_r^2 - r^{-1}\partial_r - r^{-2}\partial_\theta^2 + 1. \tag{A.16}$$

Proposition A.7. *(i) Let w satisfy equation* (A.1) *in X. Then*

$$\mathcal{I}(\beta) := \int_{\mathcal{Y}_\beta} \left[r^{-2} w_\theta^2 - w_r^2 - w^2 \right] rdr \tag{A.17}$$

does not depend on β.

(ii) Therefore

$$\mathcal{J}(\beta_1,\beta_2) := \iint_{\mathcal{X}_{\beta_1,\beta_2}} \left[r^{-2} w_\theta^2 - w_r^2 - w^2 \right] rdrd\theta \tag{A.18}$$

depends only on $\beta_2 - \beta_1$ and therefore is proportional to it.

Proof. One proves (i) by analyzing $-\iint_{\mathcal{X}_{\beta_1,\beta_2}} Lw \cdot \partial_\theta w \, dxdy$ (which actually was done before, since $w_\theta = -x_2 w_{x_1} + x_1 w_{x_2}$.

To prove (ii) observe that $\partial_\beta \mathcal{J}(\beta_1, \beta) = \mathcal{I}(\beta)$. □

Proposition A.8. *(i) Function*

$$\mathcal{J}(\beta_1,\beta_2) := \int_{\mathcal{X}_{\beta_1,\beta_2}} w^2 r^{-1} \, drd\theta \tag{A.19}$$

with fixed $\beta_{1,2} = \beta \mp \sigma$ is convex with respect to β (if $\sigma > 0$).

(ii) Further, if w is either symmetric or antisymmetric, then it reaches minimum as $\beta = 0$ (i.e. $\mathcal{X}_{\beta_1,\beta_2}$ is symmetric with respect to Y_0).

Proof. (i) Consider

$$0 = \iint_{\mathcal{X}_{\beta_1,\beta_2}} Lw \cdot w \, rdrd\theta = \iint_{\mathcal{X}_{\beta_1,\beta_2}} (w_r^2 + r^{-2} w_\theta^2 + w^2) \, rdrd\theta + \mathcal{I}'(\beta_1) - \mathcal{I}'(\beta_2) \tag{A.20}$$

with

$$\mathcal{I}'(\beta) = \int_{\mathcal{Y}_\beta} w w_\theta \, r^{-1} dr = \partial_\beta \mathcal{I}(\beta), \qquad \mathcal{I}(\beta) := \int_{\mathcal{Y}_\beta} w^2 \, r^{-1} dr. \tag{A.21}$$

Observe that the first term is positive. Then $\mathcal{I}'(\beta_2) - \mathcal{I}'(\beta_1) > 0$; on the other hand, it is the second derivative of $\mathcal{J}(\beta_1, \beta_2)$ with respect to β.

(ii) Moreover, for both symmetric and antisymmetric w $\mathcal{I}(\beta_2) - \mathcal{I}(\beta_1) = 0$. And the difference $\mathcal{I}(\beta_2) - \mathcal{I}(\beta_1) = 0$ for $\beta = 0$. □

Corollary A.9. *Since w_θ satisfies the same equation and is antisymmetric (symmetric) respectively, the same conclusions (i), (ii) hold for $\mathcal{J} := \int_{\mathcal{X}_{\beta_1,\beta_2}} w_\theta^2 r^{-1} \, r dr d\theta$.*

Then in virtue of Proposition A.7(ii) the same conclusions (i), (ii) hold for $\mathcal{J} := \iint_{\mathcal{X}_{\beta_1,\beta_2}} (w_r^2 + w^2) \, r dr d\theta$.

Next, observe that $L r\partial_r w = 2\Delta w = -2w$ and if we use the same arguments, as in the proof of Proposition A.8(ii) for $r\partial_r w$, then instead of the first term in (A.20) we get

$$\iint_{\mathcal{X}_{\beta_1,\beta_2}} \bigl((rw_r)_r^2 + w_{r\theta}^2 + (rw_r)^2 - w^2 \bigr) \, r dr d\theta, \tag{A.22}$$

where an additional last term appears as

$$\iint_{\mathcal{X}_{\beta_1 \beta_2}} 2w\partial_r w \cdot r^2 dr d\theta = - \iint_{\mathcal{X}_{\beta_1 \beta_2}} w^2 \, r dr d\theta.$$

Consider last two terms and skip integration by $d\theta$; plugging $w = r^{-3/2} u$ with $u(0) = 0$, we arrive to

$$\int \bigl(u_r - \frac{3}{2} r^{-1} u)^2 - r^{-2} u^2 \bigr) \, dr = \int \bigl(u_r^2 - 3r^{-1} u_r u + \frac{5}{4} r^{-2} u^2 \bigr) \, dr = \int \bigl(u_r^2 - \frac{1}{4} r^{-2} u^2 \bigr) \, dr$$

which is again nonnegative term. Then we arrive to

Corollary A.10. *The same conclusions (i) and (ii) of Proposition A.8 hold for $\mathcal{J}(\beta_1, \beta_2)$ with w replaced by rw_r, i.e. $\mathcal{J}(\beta_1, \beta_2) := \iint_{\mathcal{X}_{\beta_1,\beta_2}} w_r^2 \, r dr d\theta$.*

Then in virtue of Proposition A.7(ii) the same conclusions (i), (ii) hold for

(A.23) $$2\iint_{\mathcal{X}_{\beta_1,\beta_2}} |\partial_r w|^2\, rdrd\theta + \iint_{\mathcal{X}_{\beta_1,\beta_2}} (r^{-2}|\partial_\theta w|^2 - |\partial_r w|^2 - |w|^2|)\, rdrd\theta = \iint_{\mathcal{X}_{\beta_1,\beta_2}} (|\nabla w|^2 - |w|^2)\, dxdy.$$

Now we can prove

Proposition A.11. *Let $\alpha \in (\pi, 2\pi]$. Then for both symmetric and antisymmetric w (A.8) holds.*

Proof. Indeed, assume that it is not the case: $\iint_X (|\nabla w|^2 - w^2)\, dxdy < 0$ for some w. Then due to Corollary A.10 the same is true for X replaced by $\mathcal{X}_{\beta_1,\beta_2}$ with $\beta_{1,2} = \mp(2\pi - \alpha)/2$ and the same w. Then it is true for the sum of these to expressions (with $X == X_{-\alpha/2,\alpha/2}$ and $\mathcal{X}_{\beta_1,\beta_2}$), which is the sum of the same expressions for the half-planes $X_{\alpha/2-\pi,\alpha/2}$ and $X_{-\alpha/2,\pi-\alpha/2}$. However, for half-planes (A.8) holds. □

Let $P_\tau = \theta(\tau - \Lambda)$.

Proposition A.12. *(i) Let $\alpha \in [\pi, 2\pi]$. Then for any $\tau > 1$ for $w = Jv$, $v \in \operatorname{Ran}(I - P_\tau)$,*

(A.24) $$\|\nabla w\|^2 \ge (1+\delta)\|w\|^2$$

with $\delta = \delta(\tau) > 0$.

(ii) Let $\alpha \in (0, \pi]$. Then for any $\tau > 1$ for antisymmetric $w = Jv$, $v \in \operatorname{Ran}(I - P_\tau)$, (A.24) holds.

Proof. Observe first that

(A.25) $\{v \in \operatorname{Ran}(I - P_\tau) \colon \|v\|_Y = 1, \,:\, \|\nabla Jv\|^2 \le (1+\delta')\|Jv\|^2\}$ is a compact set in $\mathscr{L}^2(Y)$ for $\delta' = \delta'(\tau) > 0$.

Indeed, in the zone $\{x \colon |x| \ge R\}$ we can apply semiclassical arguments with $h := R^{-1}$ after scaling $x \mapsto R^{-1}x$.

Since in both cases (A.8) holds with a strict inequality for $w \ne 0$), we arrive to both Statements (i) and (ii). □

A.2 Spectrum

The above results are sufficient for our needs, for $\alpha \in (\pi, 2\pi]$. However we would like to explore the case of $\alpha \in (0, \pi)$ and even $\alpha \in (\pi, 2\pi]$ in more depth.

Corollary A.13. *(i) Let $\alpha \in [\pi, 2\pi]$. Then $\mathsf{Spec}(\Lambda) = [1, \infty)$ and it is continuous.*

(ii) Let $\alpha \in (0, \pi]$. Then $\mathsf{Spec}(\Lambda_{\mathsf{asym}}) = [1, \infty)$ and it is continuous, where Λ_{sym} and Λ_{asym} denote the restriction of Λ to the spaces of symmetric and antisymmetric functions, correspondingly.

Proof. We already know that the that essential spectrum of Λ is $[1, \infty)$. We also know that in the case (i) $\Lambda > I$ and in the case (ii) $\Lambda_{\mathsf{asym}} > I$. Therefore 1 is not an eigenvalue. Continuity of the spectrum follows from $(i[\Lambda, Q]v, v) \geq \delta \|v\|^2$ for $v \in \mathsf{Ran}(I - P_\tau)$, v is antisymmetric in the case (ii), which is due to Statements (i) and (ii) of Propostion A.12. □

Remark A.14. Paper [S-KP] is dealing mainly with the eigenvalues of Δ_2 in the planar sector under Robin boundary condition $(\partial_\nu + \gamma) w|_Y = 0$, $\gamma > 0$ [14]. Then eigenvalues τ of Λ and eigenvalues μ of that problem are related through Birman-Schwinger principle and scaling: $\mu_k = -\tau_k^{-2}\gamma^2$. Some of the results:

(i) Theorem 3.1 states that $(-\infty, -\gamma^2)$ contains only discrete spectrum of such operator and it is finite.

(ii) Theorem 2.3 states that for $\alpha \in (0, \pi)$ the bottom eigenvalue $-\gamma^2/\sin^2(\alpha/2)$ is simple and the corresponding eigenfunction is $\exp(-\gamma x_1/\sin(\alpha/2)$.

(iii) Theorem 3.6 states that for $\alpha \in [\frac{\pi}{3}, \pi)$ there is no other eigenvalues in $(0, 1)$, while Theorem 4.1 implies that the number of such eigenvalues is $\asymp \alpha^{-2}$ as $\alpha \to 0$ [15].

Then we conclude that

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[14] In that paper α is a half-angle, and ν is a unit external normal. Below we refer to this paper using our notations.

[15] In fact, the compete asymptotic expansion of the eigenvalues is derived in Theorem 4.16 of [S-KP].

Corollary A.15. *(i) Interval* $(0,1)$ *contains only discrete spectrum of* Λ_{sym} *which is finite.*

(ii) For $\alpha\in(0,\pi)$ *the bottom eigenvalues is* $\sin(\alpha/2)$ *and the corresponding eigenfunction is* $\exp(-x_1)$.

The discrete spectrum would not prevent us from the extending our main results to $\alpha\in(0,\pi)$. Even (possible) eigenvalue 1 on the edge of the essential spectrum would not be an obstacle. However eigenvalues embedded into $(1,\infty)$ are an obstacle (see Proposition A.16).

Proposition A.16. *If* $w_p = Jv_p$ *where* v_p *are eigenfunctions of* Λ, *corresponding to eigenvalues* τ_p, *and* $\tau_j=\tau_k$, *then*

$$(\nabla w_j, \nabla w_k) - (w_j, w_k) = 0. \tag{A.26}$$

In particular,

$$\|\nabla w_j, \|^2 - \|w_j\|^2 = 0. \tag{A.27}$$

Proof. It follows from equality (3.2) for $Q = x_1D_1 + x_2D_2 + i/2$ and

$$([Q,\Lambda]v_j, v_k) = (\Lambda v_j, Qv_jk) - (Qv_j, \Lambda v_k) = 0$$

for eigenfunction v_j v_k provided $\tau_j=\tau_k$. □

To extend the main sharp spectral asymptotics to operators in domains with inner edges one needs to prove the first following

Conjecture A.17. *For any* $\tau>1$ *and for any* $w=Jv$ *with symmetric* $v\in\mathsf{Ran}(I-P_\tau)$ *estimate* (A.24) *holds.*

Remark A.18. (i) Recall that this is true for $\alpha\in[\pi,2\pi]$ and, also, for $\alpha\in(0,\pi)$ and antisymmetric v. So, only the case of $\alpha\in(0,\pi)$ and symmetric v needs to be covered.

(ii) So far it is unknown, if in the the case of $\alpha\in(0,\pi)$ Λ_{sym} has eigenvalues embedded into continuous spectrum $(1,\infty)$ or on its edge.

(iii) Also it is unknown in any case, if the continuous spectrum is absolutely continuous (i.e. that the singular continuous spectrum is empty).

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To the memory of Michael Solomyak

Asymptotics of the Ground State Energy in the Relativistic Settings*,†

Victor Ivrii‡

Abstract

The purpose of this paper is to derive sharp asymptotics of the ground state energy for the heavy atoms and molecules in the relativistic settings, and, in particular, to derive relativistic Scott correction term and also Dirac, Schwinger and relativistic correction terms. Also we will prove that Thomas-Fermi density approximates the actual density of the ground state, which opens the way to estimate the excessive negative and positive charges and the ionization energy.

1 Introduction

The purpose of this paper is to derive sharp asymptotics of the ground state energy for heavy atoms and molecules in the relativistic settings, and, in particular, to derive relativistic Scott correction term and also Dirac, Schwinger and relativistic correction terms. The relativistic Scott correction term was first derived in [SSS] which both inspired our paper and provided necessary functional analytic tools; our improvement is achieved due to more refined microlocal semiclassical technique.

Also we will prove that the Thomas-Fermi density approximates the actual density of the ground state, which opens the way to estimate the excessive negative and positive charges and the ionization energy.

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In the next paper [Ivr2] we will introduce a self-generated magnetic field and improve results of [EFS2].

Multielectron Hamiltonian is given by

$$\mathsf{H} = \mathsf{H}_N := \sum_{1\le j\le N} H_{V,x_j} + \sum_{1\le j<k\le N} \frac{\mathsf{e}^2}{|x_j - x_k|} \tag{1.1}$$

on

$$\mathfrak{H} = \bigwedge_{1\le n\le N} \mathscr{H}, \qquad \mathscr{H} = \mathscr{L}^2(\mathbb{R}^3, \mathbb{C}^q) \simeq \mathscr{L}^2(\mathbb{R}^3 \times \{1,\dots,q\}, \mathbb{C}) \tag{1.2}$$

with

$$H_V = T - \mathsf{e}V(x), \tag{1.3}$$

describing N same type particles in the external field with the scalar potential $-V$ and repulsing one another according to the Coulomb law; e is the charge of the electron, T is an *operator of the kinetic energy.*

In the non-relativistic framework this operator is defined as

$$T = \frac{1}{2\mu}(-i\hbar\nabla)^2. \tag{1.4}$$

In the relativistic framework this operator is defined as

$$T = \Bigl(c^2(-i\hbar\nabla)^2 + \mu^2c^4\Bigr)^{\frac{1}{2}} - \mu^2c^4. \tag{1.5}$$

Here

$$V(x) = \sum_{1\le m\le M} \frac{Z_m\mathsf{e}}{|x - \mathsf{y}_m|} \tag{1.6}$$

and

$$d = \min_{1\le m<m'\le M} |\mathsf{y}_m - \mathsf{y}_{m'}| > 0. \tag{1.7}$$

where $Z_m\mathsf{e} > 0$ and y_m are charges and locations of nuclei.

It is well-known that the non-relativistic operator is always semibounded from below. On the other hand, it is also well-known [Herb, LY] that

Remark 1.1. One particle relativistic operator is semibounded from below if and only if

$$Z_m\beta \le \frac{2}{\pi} \qquad \forall m = 1,\dots,M; \qquad \beta := \frac{\mathsf{e}^2}{\hbar c}. \tag{1.8}$$

We will assume (1.8), sometimes replacing it by a strict inequality:

$$Z_m\beta \le \frac{2}{\pi} - \epsilon \qquad \forall m = 1, \dots, M; \qquad \beta := \frac{e^2}{\hbar c}. \tag{1.9}$$

We also assume that $d \ge CZ^{-1}$. Then we are interested in $\mathsf{E} := \inf \operatorname{Spec}(\mathsf{H})$.

Remark 1.2. (i) In the non-relativistic theory by scaling with respect to the spatial and energy variables we can make $\hbar = e = \mu = 1$ while Z_m are preserved.

(ii) In the relativistic theory by scaling with respect to the spatial and energy variables we can make $\hbar = e = \mu = 1$ while β and Z_m are preserved.

From now on we assume that such rescaling was already made and we are free to use letters $\hbar$, μ and c for other notations.

2 Functional Analytic Arguments

2.1 Estimate from below

In contrast to [SSS] we will start from the more traditional approach. We estimate $\sum_{1\le j<k\le N} \langle |x_j - x_k|^{-1}\Psi, \Psi\rangle$ from below, using Lieb's electrostatic inequality, by $\frac{1}{2}\mathsf{D}(\rho_\Psi, \Psi) - C\int \rho_\Psi^{4/3}\,dx$ where $\langle\cdot,\cdot\rangle$ means the inner product in $\mathfrak{H}$, $\rho_\Psi(x)$ is a one particle density,

$$\mathsf{D}(\rho, \rho') = \iint |x-y|^{-1}\rho(x)\rho'(y)\,dxdy,$$

and we use notations of Chapter 25.

The the standard lower estimate (25.2.2) holds:

$$\langle \mathsf{H}_N\Psi, \Psi\rangle \ge \sum_{1\le j\le N} \langle H_{V,x_j}\Psi, \Psi\rangle + \frac{1}{2}\mathsf{D}\bigl(\rho_\Psi, \rho_\Psi\bigr) - C\int \rho_\Psi^{\frac{4}{3}}(x)\,dx = \\ \sum_{1\le j\le N} \langle H_{W,x_j}\Psi, \Psi\rangle + \frac{1}{2}\mathsf{D}\bigl(\rho_\Psi - \rho, \rho_\Psi - \rho\bigr) - \frac{1}{2}\mathsf{D}\bigl(\rho, \rho\bigr) - C\int \rho_\Psi^{\frac{4}{3}}(x)\,dx, \tag{2.1}$$

where H_W is the one-particle Schrödinger operator (respectively, non-relativistic or relativistic) with the potential

$$W = V - |x|^{-1} * \rho, \tag{2.2}$$

and ρ is an arbitrary chosen real-valued non-negative function. Then again we get

$$\mathsf{E}_N \geq \operatorname{Tr}(H^-_{W+\lambda}) + \lambda N + \frac{1}{2}\mathsf{D}\bigl(\rho_\Psi - \rho, \rho_\Psi - \rho\bigr) - \frac{1}{2}\mathsf{D}\bigl(\rho, \rho\bigr) - C\int \rho_\Psi^{\frac{4}{3}}(x)\,dx \tag{2.3}$$

with arbitrary λ.

Remark 2.1. As usual, we will need to improve these estimates to recover a remainder estimate better than $O(Z^{\frac{5}{3}})$.

Now we need to prove estimate

$$\int \rho_\Psi^{\frac{4}{3}}(x)\,dx \leq CZ^{\frac{5}{3}} \tag{2.4}$$

for the ground state energy. It follows from

$$\int \rho_\Psi^{\frac{5}{3}}(x)\,dx \leq CZ^{\frac{7}{3}}, \tag{2.5}$$

equality $\int \rho_\Psi\,dx = N$ and assumption $N \lesssim Z$. To prove (2.5) we apply classical arguments of Lieb–Thirring, but replacing the Lieb–Thirring inequality by some relativistic inequalities (see Appendix A). Namely, let $\mathsf{b} := T - KU$ with $U = \rho_\Psi^{\frac{2}{3}}\varphi_< + \beta^{-1}\rho_\Psi^{\frac{1}{3}}\varphi_>$ where $\varphi_\gtrless$ is the characteristic function of $\{x\colon \rho_\Psi \gtrless \beta^{-3}\}$.

Consider the multiparticle operator $B = \sum \mathsf{b}_{x_j}$ and its lowest eigenvalue E_0. Obviously,

$$E_0 \leq \langle B\Psi, \Psi\rangle = \sum_j \langle T_{x_j}\Psi, \Psi\rangle - K\int (\rho_\Psi^{\frac{5}{3}}\varphi_< + \beta^{-1}\rho_\Psi^{\frac{4}{3}}\varphi_>)\,dx. \tag{2.6}$$

On the other hand, E_0 does not exceed the sum of negative eigenvalues of b, and due to Daubechies inequality (A.1), the absolute value of this sum does not exceed

$$C_0\int \max(U^{\frac{5}{2}}, \beta^3 U^4)\,dx \leq C_0 K^{\frac{5}{2}}\int \bigl(\rho_\Psi^{\frac{5}{3}}\varphi_< + \beta^{-1}\rho_\Psi^{\frac{4}{3}}\varphi_>\bigr)\,dx. \tag{2.7}$$

Therefore, assuming that $E_0 \leq 0$ we conclude that

$$\sum_j \langle T_{x_j}\Psi, \Psi\rangle - K\int \min(\rho_\Psi^{\frac{5}{3}}, \beta^{-1}\rho_\Psi^{\frac{4}{3}}) + C_0K^{\frac{5}{2}}\int \bigl(\rho_\Psi^{\frac{5}{3}}\varphi_< + \beta^{-1}\rho_\Psi^{\frac{4}{3}}\varphi_>\bigr)\,dx \geq 0$$

and therefore, for small positive constant K, we conclude that

$$\sum_j \langle T_{x_j}\Psi,\Psi\rangle \ge 2\epsilon_0 \int (\rho_\Psi^{\frac{5}{3}}\varphi_< + \beta^{-1}\rho_\Psi^{\frac{4}{3}}\varphi_>)\,dx. \tag{2.8}$$

Thus, we proved that for any $\Psi\in\mathfrak{H}$ (2.8) holds. Then

$$\sum_j \langle H_{x_j}\Psi,\Psi\rangle = \sum_j \langle T_{x_j}\Psi,\Psi\rangle - \int V(x)\rho_\Psi(x)\,dx \ge \\ \int \bigl(2\epsilon_0\rho_\Psi^{\frac{5}{3}} - V(x)\rho_\Psi\bigr)\varphi_<\,dx + \int \bigl(2\epsilon_0\beta^{-1}\rho_\Psi^{\frac{4}{3}} - V(x)\rho_\Psi\bigr)\varphi_>\,dx. \tag{2.9}$$

We know, that the latter expression must be less than $-c_0Z^{\frac{7}{3}}$ (it will follow, e. g., from the estimate from above). Observe that for $\ell(x)\ge aZ^{-\frac{1}{3}}$ we have $V(x) < a^{-1}Z^{\frac{4}{3}}$ and the integral over this zone of $-V\rho_\Psi$ is greater than $-C_0a^{-1}Z^{\frac{4}{3}}N$. Here and below $\ell(x) :== \min_j |x-\mathsf{y}_j|$. Let us fix a, a large enough constant.

Next,

$$\int_{\{x:\,\ell(x)\le aZ^{-1/3}\}} \bigl(\epsilon_0\rho_\Psi^{\frac{5}{3}} - V(x)\rho_\Psi\bigr)\varphi_<\,dx \ge -C\int_{\{x:\,\ell(x)\le aZ^{-1/3}\}} V^{\frac{5}{2}}\,dx \ge -C_1Z^{\frac{7}{3}}$$

and $(\epsilon_0\beta^{-1}\rho_\Psi^{1/3} - V)\varphi_>$ is positive unless $\rho_\psi > \beta^{-3}$ and $V\ge \epsilon_1\beta^{-1}\rho_\Psi^{1/3}\ge \epsilon_1\beta^{-2}$ (and then $\ell(x)\le C_0\beta$).

Therefore, we estimate $\int(\rho_\Psi^{5/3}\varphi_< + \beta^{-1}\rho_\Psi^{4/3}\varphi_<)\,dx$ from above by $CZ^{7/3}$ plus $\int_{\{x:\ell(x)\le C\beta\}} V\rho_\Psi\,dx$, and to obtain (2.4), it is sufficient to estimate this term. Further, it is sufficient to replace V by V_m (since $V=V_m+O(\beta^2)$, provided distances between nuclei are $\ge C\beta$). Also we can replace V_m by $V_m + C\beta^{-2}$.

If $Z_m\beta\le \frac{2}{\pi}-\epsilon$, then we can decompose $H=\eta(H-V^1)+(1-\eta)(H-V^0)$, where $(1-\eta)V^0$ coincides with V in the β-vicinity of y_m and equals 0 outside of the 2β-vicinity of it and $V^1=\eta^{-1}(V-(1-\eta)V^0)$, and apply all above arguments for the operator with $V=V^1$ while simply observing that $H-V^0$ is a positive operator for η sufficiently small. So we have proven that

Proposition 2.2. *Under assumption* (1.9) *for the ground state,*

$$\int \min(\beta^{-1}\rho_\Psi^{\frac{4}{3}}, \rho_\Psi^{\frac{5}{3}})\,dx \le CZ^{\frac{7}{3}} \tag{2.10}$$

and (2.4) *holds.*

Then we immediately arrive to Statement (i) below, and Statement (ii) follows from the main theorems of either [Bach] (Theorem 1) or [GS] (Theorem 3):

Corollary 2.3. *Under assumption* (1.9)

(i) The following estimate holds

$$\mathsf{E}_N \ge \mathsf{Tr}(H^-_{W+\lambda}) - \frac{1}{2}\mathsf{D}(\rho,\rho) - CZ^{\frac{5}{3}} + \frac{1}{2}\mathsf{D}(\rho-\rho_\Psi,\, \rho-\rho_\Psi), \tag{2.11}$$

where ρ, λ *are arbitrary and* $W = V - |x|^{-1} * \rho$.

(ii) Further,

$$\begin{aligned}\mathsf{E}_N \ge \mathsf{Tr}(H^-_{W+\lambda}) - \frac{1}{2}\mathsf{D}(\rho,\rho) - \\ \frac{1}{2}\int |x-y|^{-1}\,\mathsf{tr}\bigl(e^\dagger_N(x,y)\, e_N(x,y)\bigr)\,dxdy - CZ^{\frac{5}{3}-\delta} + \\ \frac{1}{2}\mathsf{D}(\rho-\rho_\Psi,\, \rho-\rho_\Psi),\end{aligned} \tag{2.12}$$

where $e_N(x,y)$ *is the Schwartz kernel of the projector to* N *lower eigestates of* H_W *and* tr *denotes the matrix trace.*

To cover[1)] the critical case[2)] we will use (2.21) from [SSS]

$$\sum_{1\le i<j\le N} |x_i - x_j|^{-1} \ge \sum_{j=1}^{N} (\rho * |x|^{-1} * \Phi_s)(x_j) - \frac{1}{2}\mathsf{D}(\rho,\rho) - CN\varepsilon^{-1}, \tag{2.13}$$

where, again, $\rho \ge 0$ is arbitrary, λ is arbitrary, $\Phi \ge 0$ is spherically symmetric with $\int \Phi\, dx = 1$, $\Phi_\varepsilon(x) = \varepsilon^{-3}\Phi(x/\varepsilon)$. Here the factor $\frac{1}{2}$ is due to the difference in notations and also now

$$W := W_\varepsilon = V - |x|^{-1} * \rho * \Phi_\varepsilon \tag{2.14}$$

instead of (2.2) and the term $-CNs^{-1}$ replaces the last term in (2.3):

---

1) Unfortunately, only partially.

2) I.e. with the non-strict inequality (1.8) instead of (1.9).

Proposition 2.4. *Under assumption* (1.8)

$$\mathsf{E}_N \ge \mathsf{Tr}(H^-_{W+\lambda}) + \lambda N - \frac{1}{2}\mathsf{D}(\rho,\rho) - CN\varepsilon^{-1}. \tag{2.15}$$

Remark 2.5. (i) Later we set $\varepsilon = Z^{-\frac{2}{3}}$. This would lead to $O(Z^{\frac{5}{3}})$ remainder estimate.

(ii) Proposition 2.4 is weaker than Corollary 2.3 in two ways: there is no improved version of corollary 2.3(ii) and also there is no "bonus term" $\frac{1}{2}\mathsf{D}(\rho-\rho_\Psi, \rho-\rho_\Psi)$ in the right-hand expression.

2.2 Estimate from above

The estimate from above is straight-forward: we simply take Ψ as a Slater determinant of N lower eigenfunctions of H_W. If there are only $N' < N$ negative eigenvalues then we take only N' such eigenvalues, because $\mathsf{E}_N \le \mathsf{E}_{N'}$. Then we arrive to

Proposition 2.6.

$$\begin{aligned}\mathsf{E}_N \le \mathsf{Tr}(H^-_{W+\lambda}) - \frac{1}{2}\mathsf{D}(\rho,\rho)+ \\ |\lambda-\nu|\cdot|\mathsf{N}^-_{W+\nu} - N| + \mathsf{D}(\operatorname{tr} e_N(x,x)-\rho,\, \operatorname{tr} e_N(x,x,\nu)-\rho) - \\ \frac{1}{2}\int |x-y|^{-1}\operatorname{tr}\bigl(e^\dagger_N(x,y)e_N(x,y)\bigr)\,dxdy\end{aligned} \tag{2.16}$$

with an arbitrary ρ *and any* $\nu \le 0$, $W = V - |x|^{-1} * \rho$.

3 Semiclassical Methods

We will need the following semiclassical expressions:

$$P'(w) = (2\pi)^{-3} q \int_{\{\xi:b(\xi)\le w\}} d\xi, \tag{3.1}$$

and its integral

$$P(w) = (2\pi)^{-3} q \int_{\{\xi:b(\xi)\le w\}} b(\xi)\, d\xi, \tag{3.2}$$

where in the non-relativistic case $b(\xi) = \frac{\hbar^2}{2\mu}|\xi|^2$ and, correspondingly for $\mu = \hbar = 1$

$$P^{\mathsf{TF}\,\prime}(w) = \frac{q}{6\pi^2} w_+^{\frac{3}{2}}, \tag{3.3}$$

$$P^{\mathsf{TF}}(w) = \frac{q}{15\pi^2} w_+^{\frac{5}{2}}, \tag{3.4}$$

while in the relativistic case $b(\xi) = (c^2\hbar^2|\xi|^2 + \mu^2 c^4)^{\frac{1}{2}} - \mu c^2$ and, correspondingly for $\mu = \hbar = 1$

$$P^{\mathsf{RTF}\,\prime}(w) = \frac{q}{6\pi^2} w_+^{\frac{3}{2}}(1 + \beta^2 w_+)^{\frac{3}{2}}. \tag{3.5}$$

Note that $P^{\mathsf{RTF}}(w)$ is an elementary function as well, and a sadistic Calculus instructor can give it on the test. However it turns out that we really do not need any separate relativistic Thomas-Fermi theory.

After scalings we have a *semiclassical zone* $\mathcal{X}_{\mathsf{scl}} := \{x\colon \ell(x) \ge cZ^{-1}\}$, where the effective semiclassical parameter is $h = 1/\zeta\ell$. Then, from the semiclassical point of view, on the energy levels ≤ 0, the relativistic operator has the same properties as the non-relativistic one.

There is also a *singular zone* $\mathcal{X}_{\mathsf{sing}} := \{x\colon \ell(x) \le cZ^{-1}\}$ and it covers the *relativistic zone* $\mathcal{X}_{\mathsf{rel}} := \{x\colon \ell(x) \le c\beta\}$. The important properties are that

$$0 \le V(x) - W(x) \le C\zeta^2 := \min(Z^{\frac{4}{3}}, Z\ell^{-1}), \tag{3.6}$$

$$|\partial^\gamma(W - V)| \le C\zeta^2 \ell(x)^{-|\gamma|} \qquad \forall \gamma : |\gamma| \le 2. \tag{3.7}$$

3.1 Trace Term

Now the rescaling methods allow us to prove the following:

Proposition 3.1. *Let condition* (1.8) *be fulfilled and let* W *satisfy* (3.6) *and* (3.7).

(i) Let $\psi_0(x)$ *be* ℓ*-admissible function*[3]*, being equal* 1 *in* $\{x\colon \ell(x) \ge 2a\}$ *and supported in* $\{x\colon \ell(x) \ge a\}$*. Then for* $W = W^{\mathsf{TF}}$

$$|\operatorname{Tr}(H^-_{W+\lambda}\psi_0) - \int P^{\mathsf{RTF}}(W + \lambda)\psi_0(x)\,dx| \le C\begin{cases} Z^{\frac{3}{2}} a^{-\frac{1}{2}} & a \le Z^{-\frac{1}{3}}, \\ Z^{\frac{5}{3}}(aZ^{\frac{1}{3}})^{-\delta} & a \ge Z^{-\frac{1}{3}}. \end{cases} \tag{3.8}$$

[3] I.e. $\partial^\alpha\psi_0| \le C_\alpha \ell^{-\alpha}$.

(ii) Let $\psi_m(x)$ *be* ℓ*-admissible, equal* 1 *in* $\{x\colon |x-\mathsf{y}_m|\le a\}$ *and supported in* $\{x\colon |x-\mathsf{y}_m|\le 2a\}$*. Then for* $W=V_m=Z_m|x-\mathsf{y}_m|^{-1}$

$$|\int \bigl(\operatorname{tr}(e^1(x,x,0)) - P^{\mathsf{RTF}}(V_m)\bigr)(1-\psi_m(x))\,dx| \le Z^{\frac{3}{2}}d^{-\frac{1}{2}}, \tag{3.9}$$

where $e^1(.,.,\tau)=\int_{-\infty}^{\tau} e(.,.,\tau')\,d\tau'$*.*

Proof. Indeed, the contribution of the ℓ-element of the partition[4] to the remainder is $O(\zeta^3\ell)$, exactly as in the non-relativistic case. Summation by partition elements results in the right-hand expression. □

Next, we need to consider vicinities of the singularities. Then the methods of Chapter 25 allow us to prove the following:

Proposition 3.2. *In the framework of Proposition 3.1 let* ϕ_m *be equal* 1 *in* $\{x\colon |x-\mathsf{y}_m|\le Z_m^{-1}\}$ *and supported in* $\{x\colon |x-\mathsf{y}_m|\le 2Z_m^{-1}\}$*. Let* $|\lambda|\le C_0Zd^{-1}$*. Then*

$$\begin{aligned} &|\operatorname{Tr}(H^-_{W+\lambda}\psi_m(1-\phi_m)) - \operatorname{Tr}(H^-_{V_m}\psi_m(1-\phi_m)) + \\ &\qquad\int \bigl(P^{\mathsf{RTF}}(W+\lambda) - P^{\mathsf{RTF}}(V_m)\bigr)\psi_m(x)(1-\phi_m(x))\,dx| \le \\ &\qquad\qquad C\begin{cases} Z^{\frac{3}{2}}d^{-\frac{1}{2}} & d\le Z^{-\frac{1}{3}},\\ Z^{\frac{5}{3}} & d\ge Z^{-\frac{1}{3}},\end{cases}\end{aligned} \tag{3.10}$$

where $d\ge cZ^{-1}$ *is the minimal distance between nuclei.*

Proof. Indeed, exactly as in the non-relativistic case, using methods of Sections 12.6 and 25.4 we estimate the contribution of an ℓ-element to the remainder by $O(\zeta\ell^3\bar{\zeta}^2\bar{\ell}^{-2})$ provided $Z^{-1+\delta}\lesssim \ell\lesssim d$, and by $O(\zeta^2\ell^2\bar{\zeta}^2)$ provided $Z^{-1}\lesssim\ell\lesssim Z^{-1+\delta}$. Here $\bar{\ell}=d$ and $\bar{\zeta}=Z^{\frac{1}{2}}d^{-\frac{1}{2}}$. This proves the required remainder estimate. For $d\le Z^{-1+\delta}$ we use a rescaling.

Summation by partition elements results in the right-hand expression. □

Remark 3.3. We need to include the cut-off $(1-\phi_m(x))$ because not only integrals of $P^{\mathsf{RTF}}(W+\lambda)$ and $P^{\mathsf{RTF}}(V_m)$ (of magnitude $\beta^3Z^4\ell^{-4}$) and $P^{\mathsf{RTF}\prime}(W+\lambda)$ are diverging at y_m, but even integral of their difference is logarithmically diverging.

[4] I.e. ℓ-admissible function $\psi(x)$, supported in $\frac{1}{2}\ell(y)$ for some y; then $\ell(x)\asymp\ell(y)$ on $\operatorname{supp}(\psi)$.

Now we need to consider CZ^{-1} vicinities of y_m and we will use the following Proposition:

Proposition 3.4. *In the framework of Proposition 3.1*

(i) $H_W \ge -C_0 Z^2$.

(ii) Further,

$$e(x,x,\lambda) \le CZ^{1-\delta}\ell(x)^{\delta-2} \qquad \text{for } |\lambda| \le c_0 Z^2. \tag{3.11}$$

Proof. (a) Assume first that $Z \asymp \beta^{-1}$ (i. e. $Z \ge \epsilon_0\beta^{-1}$); then Statement (i) follows immediately from Lieb-Yau inequality (Theorem A.2): in the operator sense $H \ge \beta^{-1}\sqrt{\Delta} - \beta^{-2} - Z_m r^{-1} \ge -\beta^{-2}$, $r = |x - \mathsf{y}_m|$.

Then $e(x,x,\lambda) \le C\ell(x)^{-3}h^{-3}$ with the semiclassical parameter h, which is $\asymp 1$ for $\ell \lesssim Z^{-1}$, $\lambda \lesssim Z^2$. Therefore,

$$e(x,x,\lambda) \le C\ell(x)^{-3} \qquad \text{for } \lambda \le C_0 Z^2,\ \ell(x) \lesssim Z^{-1}. \tag{3.12}$$

Unfortunately this estimate falls short for our needs. Let us shift $\mathsf{y}_m \mapsto 0$, and scale $x \mapsto Zx$, $\tau \mapsto Z^{-2}\tau$. Then we arrive to an operator which modulo $O(1)$ is $\sqrt{\Delta} - Zr^{-1}$. Due to

$$\sqrt{\Delta} - \frac{2}{\pi|x|} \ge A_s(\Delta)^s - B_s \tag{3.13}$$

for any $s \in [0, 1/2)$ and $A_s, B_s > 0$ we can "trade" (due to Sobolev embedding theorem) $\ell^{-1+\delta}$ by 1 in the scaled inequality (3.12) and by $Z^{1-\delta}$ in the original one, thus arriving to (3.11).

(b) Let us consider $Z \le \epsilon_0\beta^{-1}$. Observe that in the operator sense

$$H \ge (\frac{1}{4}\beta^{-2}r^{-2} + \beta^{-4})^{1/2} - Zr^{-1} - C\beta^{-2} \ge CZ^{-2};$$

the latter inequality is proven separately for $r \lesssim \beta$ and for $r \gtrsim \beta$.

Moreover, we get $H \ge \epsilon_1 \min(r^{-2}, \beta^{-1}r^{-1})$ for $r \le \epsilon_1 Z^{-1}$ and then we can trade ℓ^{-3} to CZ^3 arriving even to the stronger version of (3.12): namely,

$$e(x,x,\lambda) \le CZ^3. \tag{3.14}$$

Actually estimate (3.14) holds as $Z_m\beta \le 2\pi^{-1} - \sigma$ for $\sigma > 0$ with $C = C(\sigma)$ which could be calculated explicitly. $\square$

Then we immediately conclude that

Corollary 3.5. *In the framework of Proposition 3.1 for* $|\lambda|\le C_0 Zd^{-1}$

$$|\operatorname{Tr}(H^-_{W+\lambda}\phi_m)-\operatorname{Tr}(H^-_{V_m}\phi_m)|\le CZd^{-1}. \tag{3.15}$$

Now we can assemble all these results. However, before doing this we replace P^{RTF} by P^{TF}:

Proposition 3.6. *(i) Estimates* (3.8), (3.9) *and* (3.10) *hold with* P^{RTF} *replaced by* P^{TF}.

(ii) Estimate (3.10) *with* P^{RTF} *replaced by* P^{TF} *also holds with* $\phi_m=0$.

Proof. Statement (i) follows immediately from

$$P^{\mathsf{RTF}}(w)-P^{\mathsf{TF}}(w)\asymp\beta^2 w^{\frac{7}{2}},\qquad P^{\mathsf{RTF}\prime}(w)-P^{\mathsf{TF}\prime}(w)\asymp\beta^2 w^{\frac{5}{2}}\qquad\text{for}\ \ \beta^2 w\lesssim 1 \tag{3.16}$$

due to (3.5). Statement (ii) follows immediately from $P^{\mathsf{TF}}(w)\asymp w^{\frac{5}{2}}$, $P^{\mathsf{TF}\prime}(w)\asymp w^{\frac{3}{2}}$. ☐

Remark 3.7. Meanwhile,

$$\int\bigl(P^{\mathsf{RTF}}(V+\lambda)-P^{\mathsf{TF}}(V+\lambda)\bigr)\psi(x)\,dx\asymp\beta^2 Z^4, \tag{3.17}$$

which could be as large as Z^2.

Due to the scaling properties of $e(x,x,0)$ for $H=H_V$ and $P^{\mathsf{TF}}(V)$ for $V=V_m$ we conclude that

$$\int\bigl(\operatorname{tr}(e^1(x,x,0))-P^{\mathsf{RTF}}(V_m)\bigr)\,dx=qZ_m^2 S(Z_m\beta) \tag{3.18}$$

with an unknown function $S(Z_m\beta)$. Indeed, if $\mathsf{y}_m=0$ then $x\mapsto x/k$ transforms the operator with parameters Z_m,β into the operator with parameters $Z_m k$, βk^{-1}, multiplied by k^{-2}.

Remark 3.8. Obviously, $S(Z_m\beta)$ monotonely decreases as $\beta\to 0+$ and tends to $S(0)$ for the Schrödinger operator.

Then due to (3.9) for $V = V_m$

$$|\int \bigl(\mathsf{tr}(e^1(x,x,0)) - P^{\mathsf{TF}}(V_m)\bigr)\psi_m(x)\,dx - qZ_m^2 S(Z_m\beta)| \le Z^{\frac{3}{2}}d^{-\frac{1}{2}} \tag{3.19}$$

and we arrive to

Proposition 3.9. *Let* (1.8) *be fulfilled. Then for* $W = W^{\mathsf{TF}}$

$$|\operatorname{Tr}(H^-_{W+\lambda}) + \int P^{\mathsf{TF}}(W+\lambda)\,dx - \sum_{1\le m\le M} qZ_m^2 S(Z_m\beta)| \le C\begin{cases} Z^{\frac{3}{2}}d^{-\frac{1}{2}} & d\le Z^{-\frac{1}{3}},\\ Z^{\frac{5}{3}} & d\ge Z^{-\frac{1}{3}}.\end{cases} \tag{3.20}$$

3.2 Trace Term. II

Let improve the above results for $d \gg Z^{-\frac{1}{3}}$. Observe first that the in this case the error in (3.8) can be made $O(Z^{\frac{5}{3}}(dZ^{\frac{1}{3}})^{-\delta} + Z^{\frac{5}{3}-\delta})$ provided we include the relativistic Schwinger correction term. Since this term has magnitude $Z^{\frac{5}{3}}$ and the contributions of the zones $\{x\colon \ell(x)\le Z^{-\frac{1}{3}-\delta_1}\}$ and $\{x\colon \ell(x)\ge Z^{-\frac{1}{3}+\delta_1}\}$ in this term are $O(Z^{\frac{5}{3}-\delta})$, the difference between the relativistic and the standard non-relativistic Schwinger terms is $O(Z^{\frac{5}{3}-\delta})$, and we can use the latter

$$\mathsf{Schwinger} = (36\pi)^{\frac{2}{3}}q^{\frac{2}{3}}\int (\rho^{\mathsf{TF}})^{\frac{4}{3}}\,dx. \tag{3.21}$$

Next, consider the relativistic correction term

$$\int \Bigl(-P^{\mathsf{RTF}}(W+\lambda) + P^{\mathsf{RTF}}(V_m) + P^{\mathsf{TF}}(W+\lambda) - P^{\mathsf{TF}}(V_m)\Bigr)\psi_m(1-\phi_m)\,dx. \tag{3.22}$$

Again, one can see easily that we need to consider only the contribution of the *threshold zone* $\mathcal{Y} \coloneqq \{x\colon Z^{-\frac{1}{3}-\delta_1} \le \ell(x) \le Z^{-\frac{1}{3}+\delta_1}\}$ because the contributions of both zones $\{x\colon \ell(x)\le Z^{-\frac{1}{3}-\delta_1}\}$ and $\{x\colon \ell(x)\ge Z^{-\frac{1}{3}+\delta_1}\}$ in this term are $O(Z^{\frac{5}{3}-\delta})$.

One can see easily that in the threshold zone due to (3.5)

$$P^{\mathsf{RTF}}(w) - P^{\mathsf{TF}}(w) = \frac{q}{14\pi^2}\beta^2 w_+^{\frac{7}{2}} + O(Z^{\frac{8}{3}-\delta})$$

(for both $w=W^{\mathsf{TF}}+\lambda$ and $w=V_m$), and therefore modulo the same error expression (3.22) coincides with

$$\mathsf{RCT} := \frac{q}{14\pi^2}\beta^2\int \bigl(-(W^{\mathsf{TF}}+\lambda)_+^{\frac{7}{2}} + V^{\frac{7}{2}}\bigr)\,dx \tag{3.23}$$

with the integral taken over this zone or $\mathbb{R}^3$ (it does not matter). Then we arrive to

Proposition 3.10. *Let* (1.8) *be fulfilled and* $d\ge Z^{-\frac{1}{3}}$. *Then for* $W=W^{\mathsf{TF}}$

$$|\operatorname{Tr}(H^-_{W+\lambda}) + \int P^{\mathsf{TF}}(W+\lambda)\,dx - \sum_{1\le m\le M} qZ_m^2 S(Z_m\beta) - \mathsf{Schwinger} - \mathsf{RCT}| \le C\bigl(Z^{\frac{5}{3}}(dZ^{\frac{1}{3}})^{-\delta} + Z^{\frac{5}{3}-\delta}\bigr). \tag{3.24}$$

3.3 Trace Term. III

Obviously, all these results hold for $W=W_\varepsilon$ defined by (2.14) with $\rho=\rho^{\mathsf{TF}}$. However we need to estimate an error when we replace W_ε by W^{TF}. One can prove easily that

$$|W_\varepsilon - W^{\mathsf{TF}}| \le C_s (Z\ell^{-1})^{\frac{3}{2}}\varepsilon^2(\varepsilon\ell{-}1)^s \tag{3.25}$$

with arbitrary s for $\ell\le\epsilon_0 Z^{-\frac{1}{3}}$ and with $s=\frac{1}{2}$ for $\ell\le\epsilon_0 Z^{-\frac{1}{3}}$, and therefore,

$$|\int \bigl(P^{\mathsf{TF}}(W_\varepsilon+\lambda) - P^{\mathsf{TF}}(W^{\mathsf{TF}}+\lambda)|\,dx| \le CZ^3\varepsilon^2; \tag{3.26}$$

adding error $CZ\varepsilon^{-1}$ in (2.15) we get $C(Z^3\varepsilon^2+Z\varepsilon^{-1})$. It reaches minimum $CZ^{\frac{5}{3}}$ as $\varepsilon\asymp Z^{-\frac{2}{3}}$ and we arrive to

Proposition 3.11. *Let* (1.8) *be fulfilled. Then for* $W=W_\varepsilon$ *with* $\varepsilon=Z^{-\frac{2}{3}}$, (3.20) *holds and the left-hand expression of* (3.26) *is* $O(Z^{\frac{5}{3}})$.

3.4 N- and D-Terms

For these terms (needed for the estimate from above) arguments are simpler; let $\phi_0 = 1-\phi_1-\ldots-\phi_M$.

Proposition 3.12. *In the framework of Proposition 3.1* *(i) The following estimates hold*

$$|\int \bigl(e(x,x,\lambda) - P^{\mathsf{RTF}\prime}(W+\lambda)\bigr)\phi_0(x)\,dx| \le CZ^{\frac{2}{3}} \tag{3.27}$$

and for $d \ge Z^{-\frac{1}{3}}$

$$|\int \bigl(e(x,x,\lambda) - P^{\mathsf{RTF}\prime}(W+\lambda)\bigr)\phi_0(x)\,dx| \le C\bigl(Z^{\frac{2}{3}}(dZ^{\frac{1}{3}})^{-\delta} + Z^{\frac{2}{3}-\delta}\bigr). \tag{3.28}$$

(ii) Further,

$$|\int e(x,x,\lambda)\phi_m(x)\,dx| \le C. \tag{3.29}$$

(iii) Finally,

$$|\int \bigl(P^{\mathsf{RTF}\prime}(W+\lambda) - P^{\mathsf{TF}\prime}(W+\lambda)\bigr)\phi_0(x)\,dx| \le CZ^{\frac{1}{3}}. \tag{3.30}$$

Proposition 3.13. *In the framework of Proposition 3.1*

(i) The following estimates hold

$$\mathsf{D}\bigl((e(x,x,\lambda) - P^{\mathsf{RTF}\prime}(W+\lambda))\phi_0,\, (e(x,x,\lambda) - P^{\mathsf{RTF}\prime}(W+\lambda))\phi_0\bigr) \le CZ^{\frac{5}{3}} \tag{3.31}$$

and for $d \ge Z^{-\frac{1}{3}}$

$$\mathsf{D}\bigl((e(x,x,\lambda) - P^{\mathsf{RTF}\prime}(W+\lambda))\phi_0,\, (e(x,x,\lambda) - P^{\mathsf{RTF}\prime}(W+\lambda))\phi_0\bigr) \le CZ^{\frac{5}{3}}(dZ^{\frac{1}{3}})^{-\delta} + CZ^{\frac{5}{3}-\delta}. \tag{3.32}$$

(ii) Further,

$$\mathsf{D}\bigl(e(x,x,\lambda)\phi_m(x),\, e(x,x,\lambda)\phi_m(x)\bigr) \le CZ. \tag{3.33}$$

(iii) Finally,

$$\mathsf{D}\bigl((P^{\mathsf{RTF}\prime}(W+\lambda) - P^{\mathsf{TF}\prime}(W+\lambda))\phi_0,\, (P^{\mathsf{RTF}\prime}(W+\lambda) - P^{\mathsf{TF}\prime}(W+\lambda))\phi_0\bigr) \le CZ. \tag{3.34}$$

Proof of Propositions 3.12 and 3.13. Proof is straightforward:

Statements (i) are proven by the semiclassical scaling technique exactly as in Chapter 25.

Statements (ii) follow from Proposition 3.4. Statements (iii) follow from (3.5) and properties of W^{TF}. □

3.5 Dirac Term

Finally, consider the term $-\frac{1}{2}\iint \operatorname{tr}\bigl(e_N^\dagger(x,y)e_N(x,y)\bigr)\,dxdy$. The main contribution to it is delivered by the zone $\mathcal{Y}\times\mathcal{Y}$ where $\mathcal{Y}$ is the threshold zone, and in this zone the non-magnetic approximation delivers the correct expression

$$\mathsf{Dirac} = -\frac{9}{2}(36\pi)^{\frac{2}{3}} q^{\frac{2}{3}} \int (\rho^{\mathsf{TF}})^{\frac{4}{3}}\,dx, \tag{3.35}$$

with an error $Z^{\frac{5}{3}-\delta}$.

4 Main Theorems

Now repeating arguments of Section 25.4 we arrive to our main results:

Theorem 4.1 [5]**.** *Let assumption* (1.8) *be fulfilled. Then*

(i) The following asymptotics holds

$$\mathsf{E}_N = \mathcal{E}_N^{\mathsf{TF}} + \mathsf{Scott} + O\bigl(Z^{\frac{5}{3}} + Z^{\frac{3}{2}} d^{-\frac{1}{2}}\bigr). \tag{4.1}$$

Recall that $\mathsf{Scott} = q\sum Z_m^2 S(Z_m\beta)$ *and* d *is the minimal distance between nuclei.*

(ii) Furthermore, let assumption (1.9) *be fulfilled. Then for* $d \ge Z^{-\frac{1}{3}}$

$$\mathsf{E}_N = \mathcal{E}_N^{\mathsf{TF}} + \mathsf{Scott} + \mathsf{Dirac} + \mathsf{Swinger} + \mathsf{RCT} + O\bigl(Z^{\frac{5}{3}}(dZ^{\frac{1}{3}})^{-\delta} + Z^{\frac{5}{3}-\delta}\bigr). \tag{4.2}$$

Remark 4.2. (i) For the improved upper estimate in (4.2) we do not need assumption (1.9).

[5] Cf. Theorems 25.4.8 and 25.4.13 .

(ii) These theorems allow us to consider the free nuclei model and recover Theorem 25.4.14, albeit without assumption (1.9) we get only $\delta = 0$.

(iii) We also recover the estimate

$$|\lambda_N - \nu| \le C \begin{cases} Z^{\frac{8}{9}} & (Z-N)_+ \le Z^{\frac{2}{3}}, \\ (Z-N)_+^{\frac{1}{3}} & (Z-N)_+ \ge Z^{\frac{2}{3}}, \end{cases} \tag{4.3}$$

where ν is a chemical potential and λ_N is the N-th lowest eigenvalue of $H_{W^{\mathsf{TF}}}$ (reset to 0 if there are less than N negative eigenvalues). Furthermore, for $d \ge Z^{-\frac{1}{3}}$ one can include the factor $((dZ^{\frac{1}{3}})^{-\delta} + Z^{-\delta})$ into the right-hand expression.

Theorem 4.3 [6]**.** *Let assumption* (1.9) *be fulfilled. Then*

(i) The following estimate holds:

$$\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}}, \rho_\Psi - \rho^{\mathsf{TF}}) \le CZ^{\frac{5}{3}}. \tag{4.4}$$

(ii) Furthermore, for $d \ge Z^{-\frac{1}{3}}$

$$\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}}, \rho_\Psi - \rho^{\mathsf{TF}}) \le C(Z^{\frac{5}{3}}(dZ^{\frac{1}{3}})^{-\delta} + Z^{\frac{5}{3}-\delta}). \tag{4.5}$$

Remark 4.4. (i) Estimates (4.4) and (4.5) allow us to consider the excessive negative charge and ionization energy and, repeating arguments of Section 25.5, to recover Theorems 25.5.2 and 25.5.3.

(ii) Further, these estimates allow us to consider the excessive positive charge in the free nuclei model and, repeating arguments of Section 25.6, to recover Theorems 25.6.3 and 25.6.4.

Remark 4.5. We can even make a poor man version of (4.2) in the critical case, when only assumption (1.8) is fulfilled.

(i) Consider how our terms depend on q. In the atomic case consider given Z, N and shift to $\mathsf{y}_1 = 0$. Then

$$\rho_q^{\mathsf{TF}}(x) = q^2 \rho_1^{\mathsf{TF}}(q^{\frac{2}{3}} x), \qquad W_q^{\mathsf{TF}}(x) = q^{\frac{2}{3}} W_1^{\mathsf{TF}}(q^{\frac{2}{3}} x) \tag{4.6}$$

and $\mathcal{E}^{\mathsf{TF}} \asymp q^{\frac{2}{3}} Z^{\frac{7}{3}}$, $\mathsf{Scott} \asymp qZ^2$, $\mathsf{Dirac} \asymp \mathsf{Schwinger} \asymp q^{\frac{4}{3}} Z^{\frac{5}{3}}$, while $\mathsf{RCT} \asymp q^{\frac{4}{3}} \beta^2 Z^{\frac{11}{3}}$.

[6] Cf. Theorem 25.4.15.

(ii) Repeating the corresponding arguments in [SSS], one can prove that in the correlation inequality (2.13), the constant is $C(q) \le C_0 q^{\frac{2}{3}}$. On the other hand, we use the estimate for $|W - W_\varepsilon| \asymp q\varepsilon^2 Z^{\frac{3}{2}} \ell^{-\frac{3}{2}}$ and then the approximation error is $C_0 Z^3 q^2 \varepsilon^2$. Optimizing $Z^3 q^2 \varepsilon^2 + Z q^{\frac{2}{3}} \varepsilon^{-1}$ by ε we get $C q^{\frac{10}{9}} Z^{\frac{5}{3}}$ and for a large constant q it is less than $q^{\frac{4}{3}}$. In the "real life" $q = 2$.

A Some Inequalities

We follow [SSS] with some modifications:

The following two inequalities we recall are crucial in many of our estimates. They serve as replacements for the Lieb-Thirring inequality [LT] used in the non-relativistic case.

Theorem A.1 (Daubechies inequality). *(i) One-body case:*

$$\operatorname{Tr}\bigl[(\beta^{-2}\Delta + \beta^{-4})^{\frac{1}{2}} - \beta^{-2} - V(x)\bigr]^{-} \ge -C \int \Bigl(V_+^{(n+2)/2} + \beta^n V_+^{n+1}\Bigr)\,dx. \tag{A.1}$$

where $n \ge 3$ is a dimension.

(ii) Many-body case: Let $\Psi \in \bigwedge_{j=1}^{N} \mathscr{L}^2(\mathbb{R}^3;\mathbb{C}^q)$ and let ρ_Ψ be its one-particle density. Then for $n = 3$

$$\langle \sum_{j=1}^{N} \bigl[(\beta^{-2}\Delta_j + \beta^{-4})^{\frac{1}{2}} - \beta^{-2}\bigr]\Psi, \Psi\rangle \ge \int \min\bigl(\rho_\Psi^{\frac{5}{3}}, \beta^{-1}\rho_\Psi^{\frac{4}{3}}\bigr)\,dx. \tag{A.2}$$

This theorem also holds in the non-relativistic limit $\beta = 0$ and operator $(\beta^{-2}\Delta + \beta^{-4})^{\frac{1}{2}} - \beta^{-2}$ replaced by $\frac{1}{2}\Delta$.

Theorem A.2 (Lieb-Yau inequality). *Let $n = 3$. Let $C > 0$ and $R > 0$ and let*

$$H_{C,R} = \Delta^{\frac{1}{2}} - \frac{2}{\pi|x|} - C/R. \tag{A.3}$$

Then, for any density matrix γ and any function θ with support in $B_R = \{x \mid |x| \le R\}$

$$\operatorname{Tr}\bigl[\bar{\theta}\gamma\theta H_{C,R}\bigr] \ge -4.4827\, C^4 R^{-1}\{3/(4\pi R^3) \int |\theta(x)|^2\,dx\}. \tag{A.4}$$

Note that when $\theta = 1$ on B_R then the term inside the brackets $\{\}$ equals 1.

Theorem A.3 (Critical Hydrogen inequality). *Let* $n = 3$. *For any* $s \in [0, 1/2)$ *there exists constants* $A_s, B_s > 0$ *such that*

$$\Delta^{\frac{1}{2}} - \frac{2}{\pi|x|} \geq A_s \Delta^s - B_s. \tag{A.5}$$

Theorem A.4 (Hardy-Littlewood-Sobolev inequality). *There exists a constant* C *such that*

$$\mathsf{D}(f) := \iint |x - y|^{-1} f(x) f^\dagger(y)\, dxdy \leq C \, \|f\|^2_{\mathscr{L}^{6/5}}. \tag{A.6}$$

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Asymptotics of the ground state energy in the relativistic settings and with self-generated magnetic field*,†

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Abstract

The purpose of this paper is to derive sharp asymptotics of the ground state energy for the heavy atoms and molecules in the relativistic settings, with the self-generated magnetic field, and, in particular, to derive relativistic Scott correction term and also Dirac, Schwinger and relativistic correction terms. Also we will prove that Thomas-Fermi density approximates the actual density of the ground state, which opens the way to estimate the excessive negative and positive charges and the ionization energy.

1 Introduction

Multielectron Hamiltonian is defined by

$$\mathsf{H}=\mathsf{H}_N:=\sum_{1\le j\le N} H_{V,x_j}+\sum_{1\le j<k\le N}\frac{\mathsf{e}^2}{|x_j-x_k|} \tag{1.1}$$

on

$$\mathfrak{H}=\bigwedge_{1\le n\le N}\mathscr{H},\qquad \mathscr{H}=\mathscr{L}^2(\mathbb{R}^3,\mathbb{C}^q)\simeq\mathscr{L}^2(\mathbb{R}^3\times\{1,\dots,q\},\mathbb{C}) \tag{1.2}$$

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with

$$H_V = T - \mathsf{e}V(x), \tag{1.3}$$

describing N same type particles in the external field with the scalar potential $-V$ and repulsing one another according to the Coulomb law; e is a charge of the electron, T is an *operator of the kinetic energy*. Unless specifically mentioned, $q = 2$.

In the non-relativistic framework this operator is defined as

$$T = \frac{1}{2\mu}(-i\hbar\nabla - \mathsf{e}A)^2, \tag{1.4$_1$}$$

$$T = \frac{1}{2\mu}\bigl((i\nabla - \mathsf{e}A)\cdot\boldsymbol{\sigma}\bigr)^2 \tag{1.4$_2$}$$

in the magnetic (Schrödinger) and (Schrödinger-Pauli) settings respectively.

In the relativistic framework this operator is defined as

$$T = \Bigl(c^2(-i\hbar\nabla - \mathsf{e}A)^2 + \mu^2c^4\Bigr)^{\frac{1}{2}} - \mu^2c^4 \tag{1.5$_1$}$$

$$T = \Bigl(c^2\bigl((-i\hbar\nabla - \mathsf{e}A)\cdot\boldsymbol{\sigma}\bigr)^2 + \mu^2c^4\Bigr)^{\frac{1}{2}} - \mu^2c^4 \tag{1.5$_2$}$$

in the magnetic (Schrödinger) and (Schrödinger-Pauli) settings respectively.

Recall that in non-magnetic settings we have (1.4) and (1.5) of [Ivr2] in the non-relativistic and relativistic settings respectively. Here

$$V(x) = \sum_{1\le m\le M} \frac{Z_m\mathsf{e}}{|x - \mathsf{y}_m|} \tag{1.6}$$

and

$$d = \min_{1\le m<m'\le M} |\mathsf{y}_m - \mathsf{y}_{m'}| > 0. \tag{1.7}$$

where $Z_m\mathsf{e} > 0$ and y_m are charges and locations of nuclei.

It is well-known that the non-relativistic operator is always semibounded from below. On the other hand, it is also well-known [Herb, LY] that one particle relativistic non-magnetic operator is semibounded from below if and only if $Z_m\beta \le \frac{2}{\pi}$ for $m = 1, \dots, M$. In this paper we assume a strict condition:

$$Z_m\beta \le \frac{2}{\pi} - \epsilon \qquad \forall m = 1, \dots, M; \qquad \beta := \frac{\mathsf{e}^2}{\hbar c}. \tag{1.8}$$

In the non-magnetic case we were interested in $\mathsf{E} := \inf\operatorname{Spec}(\mathsf{H})$. In the magnetic case we consider only a self-generated magnetic field, that is we consider

$$\mathsf{E}^* = \inf_{A\in\mathscr{H}^1_0} \mathsf{E}(A), \tag{1.9}$$

where

$$\mathsf{E}(A) = \inf\operatorname{Spec}(\mathsf{H}_{A,V}) + \underbrace{\frac{\mathsf{e}^2}{\alpha\hbar^2}\int |\nabla\times A|^2\,dx}, \tag{1.10}$$

$$\alpha Z_m \le \kappa^*(2\pi^{-1} - \beta Z_m)^{\frac{3}{2}} \qquad m = 1,\dots,M. \tag{1.11}$$

with a unspecified constant $\kappa^* > 0$. We also assume that $d \ge CZ^{-1}$.

Remark 1.1. (i) In the non-relativistic theory by scaling with respect to the spatial and energy variables we can make $\hbar = \mathsf{e} = \mu = 1$ while α and Z_m are preserved.

(ii) In the relativistic theory by scaling with respect to the spatial and energy variables we can make $\hbar = \mathsf{e} = \mu = 1$ while β, α and Z_m are preserved.

(iii) In the one particle case there are additional scalings with respect to the spatial and energy variables, preserving only $Z_m\alpha$ and $Z_m\beta$ (but not the Z_m, α, β).

From now on we assume that such rescaling was done and we are free to use letters $\hbar$, μ and c for other notations.

The sharp results in the non-relativistic frameworks, without magnetic field and with self-generated magnetic filed were obtained in Chapters 25 and 27 respectively, and in the relativistic frameworks without magnetic field—in [Ivr2]. The transition from the non-relativistic framework to the relativistic one required mainly modifications of the function-analytic arguments in the *singular zone* $\bigcup_m\{x\colon |x-\mathsf{y}_m| \le cZ_m^{-1}\}$, and it was done in many articles, listed in the references, which we heavily use. On the other hand, transition from the non-magnetic case to the case of the self-generated magnetic field requires microlocal semiclassical arguments of Chapter 27 in the *semiclassical zone* $\bigcap_m\{x\colon |x-\mathsf{y}_m| \ge cZ_m^{-1}\}$, which we also heavily rely upon. However relativistic settings require modifications of these arguments, and we are providing most of details when such modifications are needed, and are rather sketchy when no modifications are required.

2 Local Semiclassical Trace Asymptotics

2.1 Set-up

This section matches to Section 27.2. We consider potential W supported in $B(\mathsf{x},r)$ (with $r=\ell(\mathsf{x})$ the half-distance to the nearest nucleus), and scale it to $B(0,1)$ with $W\asymp 1$.

Recall that the original non-relativistic operator is

$$\frac{1}{2}((D-A)\cdot\boldsymbol{\sigma})^2 - W, \tag{2.1}$$

which after rescaling $x\mapsto (x-\mathsf{x})/r$, $\tau\mapsto\tau/(Zr^{-1})$ becomes

$$\frac{1}{2}((hD-A')\cdot\boldsymbol{\sigma})^2 - W,\qquad h=Z^{-1/2}r^{-1/2},\qquad A'=Z^{-1/2}r^{1/2}A, \tag{2.2}$$

while the "penalty" becomes

$$\frac{r}{\alpha}\int |\nabla\times A'|^2\,dx = \frac{1}{\kappa h^2}\int |\nabla\times A'|^2\,dx \tag{2.3}$$

with $\kappa=Z\alpha$ and we assume that $\kappa\le\kappa^*$.

What happens with our relativistic operator? The same scaling transforms $\bigl(\beta^{-2}((D-A)\cdot\boldsymbol{\sigma})^2+\beta^{-4}\bigr)^{1/2}-\beta^{-2}$ into

$$\begin{aligned} rZ^{-1}\bigl(\beta^{-2}((r^{-1}D-A)\cdot\boldsymbol{\sigma})^2+\beta^{-4}\bigr)^{1/2} - rZ^{-1}\beta^{-2} =\\ \bigl(\gamma^{-2}((hD-A')\cdot\boldsymbol{\sigma})^2+\gamma^{-4}\bigr)^{1/2}-\gamma^{-2}\end{aligned} \tag{2.4}$$

with $\gamma=\beta h^{-1}\le 1$.

Exactly like in Subsubsection 27.2.1 we need to start with the functional-analytic arguments.

2.2 Functional Analytic Arguments

Estimates

Proposition 2.1 [1]**.** *Let* $V\in\mathscr{L}^{\frac{5}{2}}\cap\mathscr{L}^4$*. Then*

$$\mathsf{E}^*\ge -Ch^{-3} \tag{2.5}$$

[1] Cf. Proposition 27.2.1.

and either

$$\frac{1}{\kappa h^2}\int |\partial A|^2\,dx \le Ch^{-3} \tag{2.6}$$

or $\mathsf{E}(A) \ge ch^{-3}$.

Proof. Using Theorem A.1 (magnetic Daubechies inequality rather than magnetic Lieb-Thirring inequality) with $\gamma := \gamma h$, $V := h^{-2}V$, $A := h^{-1}A$ and with multiplication of the result by h^2, we have

$$\begin{multline}\operatorname{Tr}(H^-_{A,V}) \ge \\ - Ch^{-3}\int \Bigl(V_+^{5/2} + \gamma^3 V_+^4\Bigr)\,dx - Ch^{-2}\Bigl(|\partial A|^2\,dx\Bigr)^{\frac{1}{4}}\Bigl(V_+^4\,dx\Bigr)^{\frac{3}{4}}\end{multline} \tag{2.7}$$

(cf. (27.2.9); only the term $\gamma^3 V_+^4$ adds up); then (27.2.10) holds, which completes the proof. □

Proposition 2.2 [2]**.** *Let* $V_+ \in \mathscr{L}^{\frac{5}{2}} \cap \mathscr{L}^4$, $\kappa \le ch^{-1}$ *and*

$$V \le -C^{-1}(1+|x|)^{\delta} + C. \tag{2.8}$$

Then there exists a minimizer A.

Proof. Let us consider a minimizing sequence A_j. Without any loss of the generality one can assume that $A_j \to A_\infty$ weakly in $\mathscr{H}^1$ and in $\mathscr{L}^6$ and then strongly in $\mathscr{L}^p_{\mathsf{loc}}$ with any $p < 6$ [3]. Then A_∞ is a minimizer.

Really, due to (2.6) and (2.8) negative spectra of $H_{A_j,V}$ are discrete and the number of negative eigenvalues is bounded by $N = N(h)$. Consider ordered eigenvalues $\lambda_{j,k}$ of $H_{A_j,V}$. Without any loss of the generality one can assume that $\lambda_{j,k}$ have limits $\lambda_{\infty,k} \le 0$ (we go to the subsequence if needed).

We claim that $\lambda_{\infty,k}$ are also eigenvalues and if $\lambda_{\infty,k} = \dots = \lambda_{\infty,k+r-1}$ then it is eigenvalue of at least multiplicity r.

Indeed, let $u_{j,k}$ be corresponding eigenfunctions, orthonormal in $\mathscr{L}^2$. Then in virtue of A_j being bounded in $\mathscr{L}^6$ and $V \in \mathscr{L}^4$ we can estimate

$$\||D|^{1/2}u_{j,k}\| \le K\|u_{j,k}\|_6^{1-\delta}\cdot\|u_{j,k}\|^{\sigma} \le K\||D|^{1/2}u_{j,k}\|^{1-\delta}\cdot\|u_{j,k}\|^{\delta}$$

[2] Cf. Proposition 27.2.2.

[3] Otherwise we select a converging subsequence.

with $\delta > 0$ which implies $\||D|^{1/2}u_{j,k}\| \le K$. Also assumption (2.8) implies that $\|(1+|x|)^{\delta/2}u_{j,k}\|$ are bounded and therefore without any loss of the generality one can assume that $u_{j,k}$ converge strongly.

Then

$$\lim_{j\to\infty} \mathsf{Tr}(H^-_{A_j,V}) \ge \mathsf{Tr}(H^-_{A_\infty,V}), \tag{2.9}$$

$$\liminf_{j\to\infty} \int |\partial A_j|^2\,dx \ge \int |\partial A_\infty|^2\,dx \tag{2.10}$$

and therefore $\mathsf{E}(A_\infty) \le \mathsf{E}^*$. Then A_∞ is a minimizer and there are equalities in (2.9)–(2.10) and, in particular, there no negative eigenvalues of $H_{A_\infty,V}$ other than $\lambda_{\infty,k}$. □

Properties of a Minimizer

Next, we need to study the minimizer[4].

Proposition 2.3 [5]**.** *Let A be a minimizer. Then*

$$\begin{aligned}\frac{2}{\kappa h^2}\Delta A_j(x) = \Phi_j :=\\ &- \operatorname{Re}\operatorname{tr}\Bigl[\int_0^\infty \sigma_j((hD-A)_x\cdot\boldsymbol{\sigma})e^{-\lambda S}e(.,.,0)e^{-\lambda S}\,d\lambda\Bigr]\Bigr|_{x=y}\\ &- \operatorname{Re}\operatorname{tr}\Bigl[\int_0^\infty \sigma_j e^{-\lambda S}e(.,.,0)e^{-\lambda S}\,{}^t((hD-A)_y\cdot\boldsymbol{\sigma})\,d\lambda\Bigr]\Bigr|_{x=y}.\end{aligned} \tag{2.11}$$

where $A=(A_1,A_2,A_3)$, $\boldsymbol{\sigma}=(\sigma_1,\sigma_2,\sigma_3)$ and $e(x,y,\tau)$ is the Schwartz kernel of the spectral projector $\theta(-H)$ of $H=H_{A,V}$ and tr is a matrix trace;

$$S=\gamma^2(T+\gamma^{-2}) = \bigl((\gamma^2(hD-A)\cdot\boldsymbol{\sigma})^2+1\bigr)^{\frac{1}{2}} \tag{2.12}$$

Proof. Consider variation δA of A and variation of $\mathsf{Tr}(H^-)$ where $H^- = H\theta(-H)$ is a negative part of H. Then, like in the proof of Proposition 27.2.4,

$$\delta\,\mathsf{Tr}(H^-) = \mathsf{Tr}\bigl((\delta H)\theta(-H)\bigr). \tag{2.13}$$

[4] We do not know if it is unique, exactly like in the non-relativistic case; see Remark 27.2.3.

[5] Cf. Proposition 27.2.4. Observe that (2.11) is more complicated than (27.2.14).

But we need to find $\delta H = \gamma^{-2}\delta S$, which is a bit more tricky than in the non-relativistic case. Observe that

$$\delta(S^2) = S(\delta S) + (\delta S)S; \tag{2.14}$$

then

$$\delta S = \int_0^\infty e^{-\lambda S}\delta(S^2)e^{-\lambda S}\,d\lambda \tag{2.15}$$

while

$$\gamma^{-2}S^2 = ((hD - A)\cdot\boldsymbol{\sigma})^2 + \gamma^{-2} \tag{2.16}$$

and therefore

$$\delta(\gamma^{-2}S^2) = -\sum_j \Bigl(\delta A_j\sigma_j((hD-A)\cdot\boldsymbol{\sigma}) - ((hD-A)\cdot\boldsymbol{\sigma})\delta A_j\sigma_j\Bigr), \tag{2.17}$$

exactly like in non-relativistic case.

Therefore $\operatorname{Tr}(\delta S\theta(-H))$ is equal to the sum of $\int_0^\infty d\lambda$ of

$$\begin{aligned}
&-\operatorname{Tr}\Bigl(e^{-\lambda S}\delta A_j\sigma_j((hD-A)\cdot\boldsymbol{\sigma})e^{-\lambda S}\theta(-H)\Bigr)\\
&-\operatorname{Tr}\Bigl(e^{-\lambda S}((hD-A)\cdot\boldsymbol{\sigma})\delta A_j\sigma_j e^{-\lambda S}\theta(-H)\Bigr) =\\
&-\operatorname{Tr}\Bigl(\delta A_j\sigma_j((hD-A)\cdot\boldsymbol{\sigma})e^{-tS}\theta(-H)e^{-\lambda S}\Bigr)\\
&-\operatorname{Tr}\Bigl(\delta A_j\sigma_j e^{-\lambda S}\theta(-H)e^{-\lambda S}((hD-A)\cdot\boldsymbol{\sigma})\Bigr).
\end{aligned}$$

Then $\operatorname{Tr}(\delta L\theta(-H)) = \int\sum_j \Phi_j(x)\delta A_j$, which implies equality (2.11). □

Proposition 2.4 [6]**.** *If for $\kappa = \kappa^*$*

$$\mathsf{E}^* \ge \mathsf{Weyl}_1 - CM \tag{2.18}$$

(2.19)

with $M \ge Ch^{-1}$, then for $\kappa \le \kappa^*(1-\epsilon_0)$

$$\frac{1}{\kappa h^2}\int |\partial A|^2\,dx \le C_1 M. \tag{2.20}$$

[6] Cf. Proposition 27.2.5.

Proof. Proof is obvious, also based on the upper estimate $\mathsf{E}^* \le \mathsf{E}(0) \le \mathsf{Weyl}_1 + Ch^{-1}$, which is due to [Ivr2]. □

Proposition 2.5 [7]**.** *Let estimate* (2.20) *be fulfilled and let*

$$\varsigma = \kappa M h \le c. \tag{2.21}$$

Then for $\tau \le c$

(i) Operator norm in $\mathscr{L}^2$ *of* $(hD)^k\theta(\tau - H)$ *does not exceed* C *for* $k = 0, 1$.

(ii) Operator norm in $\mathscr{L}^2$ *of* $(hD)^k\bigl((hD - A)\cdot\boldsymbol{\sigma}\bigr)\theta(\tau - H)$ *does not exceed* C *for* $k = 0$.

Proof. First, let us repeat of some arguments of the proof of Proposition 27.2.6. Let $u = \theta(\tau - H)f$. Then $\|u\| \le \|f\|$ and since

$$\|A\|_{\mathscr{L}^6} \le C\|\partial A\| \le C(\kappa M)^{\frac{1}{2}} h, \tag{2.22}$$

we conclude that

$$\begin{aligned}\|hDu\| \le \|(hD - A)u\| + \|Au\| \le \|(hD - A)u\| + C\|A\|_{\mathscr{L}^6}\cdot\|u\|_{\mathscr{L}^3} \le \\ \|(hD - A)u\| + C(\kappa M)^{\frac{1}{2}} h\|u\|^{1/2}\cdot\|u\|_{\mathscr{L}^6}^{1/2} \le \\ \|(hD - A)u\| + C(\kappa M h)^{\frac{1}{2}}\|u\|^{1/2}\cdot\|hDu\|^{1/2} \le \\ \|(hD - A)u\| + \frac{1}{2}\|hDu\| + C\kappa M h\|u\|;\end{aligned}$$

therefore due to (2.21)

$$\|hDu\| \le 2\|(hD - A)u\| + C\kappa M h\|u\|. \tag{2.23}$$

Further, $\|Tu\| \le c_1\|u\|$ because $H \ge -c$, $|V| \le c$, $|\tau| \le c$; then $\|(T + \gamma^{-2})u \le (c_1 + \gamma^{-2})\|u\|$ and therefore

$$(((T + \gamma^{-2})^2 - \gamma^{-4})u, u) \le ((c_1 + \gamma^{-2})^2 - \gamma^{-4}) = (2c_1\gamma^{-2} + c_1^2)\|u\|^2,$$

and finally

$$(Lu, u) \le C\|u\|^2 \tag{2.24}$$

[7] Cf. Proposition 27.2.6.

with

$$L := ((hD - A)\cdot \boldsymbol{\sigma})^2. \tag{2.25}$$

Then, again following the same proof, we conclude that

$$\|(hD - A)u\| \le C\|u\| \quad \text{and} \quad \|hDu\| \le C(1 + \kappa Mh)\|u\|, \tag{2.26}$$

provided $\kappa Mh^{1+\delta} \le c$ for sufficiently small $\delta > 0$. Therefore under assumption (2.21) for $j = 0, 1$ both Statements (i) and (ii) are proven. □

Thus, in contrast to Proposition 27.2.6 of, we do not have $k = 2$ in Statement (i), and $k = 1$ in Statement (ii) so far and need some extra arguments.

Proposition 2.6. *Assume that* $\|V\|_{\mathscr{C}^2} \le c$. *Then*

$$\|[S, V]u\| \le Ch\gamma^2(\|L^{\frac12}u\| + \|u\|). \tag{2.27}$$

Proof. Recall that that $S^2 = \gamma^2 L + 1$. Therefore $\gamma^2[L, V] = [S, V]S + S[S, V]$ and then

$$[S, V] = \gamma^2 \int_0^\infty e^{-\lambda S}[L, V]e^{-\lambda S}\, d\lambda. \tag{2.28}$$

Also

$$\|[L, V]w\| \le Ch(\|L^{1/2}w\| + \|w\|) \tag{2.29}$$

and

$$\|e^{-\lambda S}\| \le e^{-\lambda}. \tag{2.30}$$

Proposition 2.7. *(i) Assume that* $\|V\|_{\mathscr{C}^2} \le c$ *and* $|\tau| \le c$. *Then the operator norm of* $(hD)^k\theta(\tau - H)$ *does not exceed* C *for* $k = 0, 1, 2$.

(ii) Assume that $\|V\|_{\mathscr{C}^3} \le c$ *and* $|\tau| \le c$. *Then the operator norm of operators* $(hD)^k((hD - A)_x \cdot \boldsymbol{\sigma})\theta(\tau - H)$ *and* $(hD)^k\hat{\Phi}_j\theta(\tau - H)$ *with*

$$\hat{\Phi}_j = \int_0^\infty \sigma_j((hD - A)_x \cdot \boldsymbol{\sigma})e^{-\lambda S}e(.,.,0)e^{-\lambda S}\, d\lambda \tag{2.31}$$

do not exceed C *for* $k = 0, 1, 2$.

Proof. (i) Let $u=\theta(\tau-H)f$ with $f\in\mathscr{L}^2$. Then u satisfies (2.2) and $\|Tu\|\le C\|u\|$. Also, which implies

$$\gamma^{-2}\|Lu\|=\|(T+2\gamma^{-2})Tu\|\le C\gamma^{-2}\|u\|+C\gamma^{-1}\|[T,V]u\|\le C_1\gamma^{-2}\|u\|$$

due to (2.27) . Then, repeating arguments of the proof of Propositiob 27.2.6, we conclude that $\|(hD)^2u\|\le C\|u\|$, i.e. Statement (i).

(ii) Plugging $(T-V-\tau)u$ instead of u (with $\|(T-V-\tau)u\|\le C\|u\|$) we have $\|L(T-\tau-V)u\|\le C\|u\|$. Then

$$\|TLu\|\le C\|Lu\|+C\|[L,V]u\|\le C(\|Lu\|+\|u\|)\le C_1\|u\|.$$

Again plugging $(T-V-\tau)u$ instead of u we have

$$\gamma^{-2}\|L^2u\|=\|(T+2\gamma^{-2})TLu\|\le \\ \|T(T-V-\tau)Lu\|\le C\gamma^{-2}\|Lu\|+C\|T[L,V]u\|.$$

Further, the last term does not exceed $Ch\|TV'L^{\frac{1}{2}}u\|+Ch^2\|TV''u\|$ where V' are miscellaneous first derivatives of V and $V''=\Delta V$. Then, the former does not exceed $C\|Lu\|$, while the latter does not exceed $C\gamma^{-2}\|u\|+h\|\nabla(V''u)\|$, which does not exceed $C\gamma^{-2}\|u\|$.

Therefore $\|L^2u\|\le C\|u\|$, which implies that $\|L((hD-A)\cdot\boldsymbol{\sigma})u\|\le C\|u\|$, which in turn implies that $\|(hD)^2((hD-A)\cdot\boldsymbol{\sigma})u\|\le C\|u\|$ and, finally, $\|(hD)^2\hat{\Phi}_ju\|\le C\|u\|$. □

Corollary 2.8. *(i) Assume that $\|V\|_{\mathscr{C}^2}\le c$ and $|\tau|\le c$. Then the operator norm of $\theta(\tau-H)$ from $\mathscr{L}^2$ to $\mathscr{C}^\delta$ does not exceed $Ch^{-3/2-\delta}$ for $0\le\delta\le\frac{1}{2}$.*

(ii) Assume that $\|V\|_{\mathscr{C}^3}\le c$ and $|\tau|\le c$. Then the operator norm of $\hat{\Phi}_j$ from $\mathscr{L}^2$ to $\mathscr{C}^\delta$ do not exceed $Ch^{-3/2-\delta}$ for $0\le\delta\le\frac{1}{2}$. Then $\|\Phi_j\|_{\mathscr{C}}\le Ch^{-3}$.

Corollary 2.9. *Under assumptions* (2.18)–(2.21) $\|A_j\|_{\mathscr{C}^{2-\delta}}\le C\kappa h^{-1}$ *for any $\delta>0$.*

2.3 Microlocal Analysis and Local Theory

Microlocal Analysis Unleashed

Then we can apply all arguments of Subsection 27.2.2[8], even if expression for Φ_j differs. Indeed, observe first that we can restrict ourselves by $0 \le \lambda \le c|\log h|$. Then, using our standard arguments based on the analysis of the propagation of singularities, we can prove that the Tauberian expression with $T = h^{1-\delta}$ for Φ_j has an error $O(h^{-2})$ provided

$$V(x) \asymp 1. \tag{2.32}$$

Then our standard trick with the freezing coefficients works and with the same $O(h^{-2})$ error we can replace $\Phi_j(x)$ by its Weyl expression, i.e. expression we obtain if replace operators by their symbols, depending on x and ξ, integrating by $d\xi$ and multiplying by $(2\pi h)^{-3}$. However due to skew-symmetry with respect to $\xi - A(x)$, this Weyl expression is 0, and $\Phi_j(x) = O(h^{-2})$.

Finally, we can get rid of assumption (2.32) by the standard rescaling arguments. We leave all the details to the reader.

Local Theory and Rescaling

Then we can apply all arguments of Subsection 27.2.3 [9]. As a result we arrive under assumption (2.21) to the trace formula[10] with the remainder estimate $O(h^{-1})$ and to estimate $\|\partial A\| = O(\kappa^{1/2}h^{1/2})$.

Moreover, under the standard assumption of the global nature we arrive to the trace formula with the remainder estimate $o(h^{-1})$ (but it will have the Schwinger-type correction term) and to estimate $\|\partial A\| = o(\kappa^{1/2}h^{1/2})$.

Finally, we an apply all arguments of Subsection 27.2.4 [11] and we weaken assumption (2.21), recovering the same estimates as before. Again, we leave all the details to the reader.

---

[8] Namely of Subsubsections *27.2.2.1. Sharp Estimates*, *27.2.2.2. Application* and *27.2.2.3. Classical Dynamics and Sharper Estimates.*

[9] Namely, Subsubsections *27.2.3.1. Localization and Estimate from above* and *27.2.3.2. Estimate from below.*

[10] In the trace formula "Weyl_1" is given by the relativistic expression, $-P^{\mathsf{RTF}}(W+\nu)$.

[11] Namely, Subsubsection *27.2.4.1. Case* $\kappa \le 1$ and Subsubsection *27.2.4.2. Case* $1 \le \kappa \le h^{-1}$.

3 Global Trace Asymptotics in the Case of Coulomb-Like Singularities

3.1 Estimates to a Minimizer

Let us return to the original settings, with Coulomb-like singularities and parameters Z_m, α, β. At the moment we consider the one-particle Hamiltonian. Let us deal first with the vicinity of y_m.

Then we scale like in Section 27.3: $x \mapsto Z^{\frac{1}{3}}x$, $\tau \mapsto Z^{-\frac{4}{3}}\tau$, $A \mapsto Z^{-\frac{2}{3}}A$, $\beta \mapsto \beta Z^{\frac{3}{3}}$, arriving to the semiclassical problem with Coulomb singularities $z_m|x - \mathsf{y}_m|^{-1}$ ($z_m = Z_m Z^{-1}$), with $h = Z^{-\frac{1}{3}}$ and with $\kappa = \alpha Z^{\frac{2}{3}}$. In particular, E^* is a minimum with respect to A of

$$\mathsf{E}(A) := \operatorname{Tr}(H^{-}_{A,W+\tau}) + \kappa^{-1}h^{-2}\|\partial A\|^2. \tag{3.1}$$

Let us follow arguments of Subsubsection *27.3.2.1 Preliminary Analysis.* Observe first that the estimate from above is

$$\mathsf{E}^* \le h^{-3}\int \mathsf{Weyl}_1(x)\,dx + Ch^{-2}; \tag{3.2}$$

we simply take $A = 0$ and refer to [Ivr2][12].

Consider now estimate from below and apply ℓ-admissible partition exactly like in Subsection 27.3.2. Then, according to the previous section, for any element of partition with $\ell \ge ch^{-2}$ ($\ell \ge cZ_m^{-1}$ in the original settings) its contribution is estimated from below by the corresponding Weyl expression minus $Ch^{-1}\zeta^2 \times \zeta\ell = Ch^{-1}\zeta^3\ell^{-1}$ and summation with respect to these elements returns $\mathcal{E}^{\mathsf{TF}}$ minus $Ch^{-1}\zeta^3\ell|_{\ell=h^{-2}}$, i.e.

$$h^{-3}\int \mathsf{Weyl}_1(x)\,dx - Ch^{-2} \tag{3.3}$$

because the contribution of the zone $\mathcal{Z}_0 = \{x\colon \ell(x) \le ch^{-2}\}$ to the main term is $O(h^{-2})$.

On the other hand, the contribution of $\mathcal{Z}_0$ is $-Ch^{-2}$. Indeed, scale first $x \mapsto h^{-2}x$, $\tau \mapsto h^2\tau$, $h \mapsto 1$, $A \mapsto hA$, $\beta \mapsto \gamma = \beta h^{-1}$, and the Coulomb

[12] In the original settings the remainder estimate would be $O(Z^2)$ exactly as in the non-relativistic case.

singularity remains the same while the magnetic energy becomes $\kappa^{-1}\|\partial A\|^2$. Observe that $\gamma=\beta_{\mathsf{orig}} Z_m$ [13], so (1.8), (1.11) become

$$\beta \le 2\pi^{-1}-\epsilon, \qquad \kappa \le \kappa^*(2\pi^{-1}-\beta). \tag{3.4}$$

Then we can apply a "singular magnetic Daubechies inequality" (A.3) and repeat all arguments of the regular case in a simple case of $h=1$. There will be an extra terms $O(1)$ and $-C(1-\pi\gamma/2)^{-\frac{3}{2}}\|\partial A\|^2$ and that latter term requires (1.11).

Now we conclude that Proposition 27.3.1 holds:

Proposition 3.1 [14]**.** *In our framework $\kappa\le\kappa^*$. Then the near-minimizer A satisfies*

$$|\int \bigl(\operatorname{tr} e_{A,1}(x,x,0) - \mathsf{Weyl}_1(x)\bigr)\,dx| \le Ch^{-2} \tag{3.5}$$

and

$$\|\partial A\| \le C\kappa^{\frac{1}{2}}. \tag{3.6}$$

It allows us to repeat arguments of the proof Proposition 2.2 and to prove

Proposition 3.2 [15]**.** *In our framework there exists a minimizer A* [4]*.*

Now we can repeat arguments of Subsubsection *27.3.2.2 Estimates to a Minimizer. I*, albeit with the right-hand expression of (27.3.14) given now by (2.11) and to prove the claim (27.3.28), which is marginally stronger than

$$\|\partial^2 A\|_{\mathscr{L}^\infty(B(0,1-\epsilon))} \le C\kappa^{\frac{1}{2}} h^{-\delta}. \tag{3.7}$$

Then we can repeat arguments of Subsubsection *27.3.2.3 Estimates to a Minimizer. II* and recover Propositions 27.3.4, 27.3.6 and 27.3.7, estimating A and its derivatives as $\ell(x)\lesssim 1$:

---

[13] Considering vicinity of y_m it is more convenient to take the original rescaling with Z replaced by Z_m, and therefore $z_m=1$.

[14] Cf. Proposition 27.3.1.

[15] Cf. Proposition 27.3.2.

Proposition 3.3 [16]**.** *In our framework if* $\ell(x) \ge \ell_* := h^2$*, then*

$$|A| \le C\kappa \ell^{-\frac{1}{2}}, \qquad |\partial A| \le C\kappa\ell^{-\frac{3}{2}} \tag{3.8}$$

and

$$|\partial A(x) - \partial A(y)| \le C_\theta \kappa \ell^{-\frac{3}{2}-\theta}|x-y|^\theta \qquad \text{as } |x-y| \le \frac{1}{2}\ell(x) \tag{3.9}$$

for any $\theta \in (0,1)$*.*

Consider now the non-semiclassical zone $\{x\colon \ell(x) \lesssim \ell_*\}$, which contains the relativistic zone $\{x\colon \ell(x) \lesssim \bar{\ell} := \gamma h\}$. Using arguments of the proof of Proposition 3.4 of [Ivr2], but additionally taking care of the magnetic field using arguments of the proofs of Propositions 2.5, 2.6 and 2.7 (we leave all details to the reader), we arrive to

Proposition 3.4. *In our framework* $H_{W,A} \ge C_0\ell_*^{-1}$ *and* $e(x,x,\lambda) \le C\ell_*^{-3}$ *for* $\ell(x) \le c\ell_*$ *and* $|\lambda| \le Ch^{-2}$*.*

Remark 3.5. (i) Then in the original settings $H_{W,A} \ge C_0 Z^{-2}$ and $e(x,x,\lambda) \le CZ^3$ for $\ell(x) \le cZ^{-1}$ and $|\lambda| \le C_0 Z^2$.

(ii) We have a better estimate than (3.11) of [Ivr2] due to assumptions (1.8) and (1.11).

Next, we follow arguments of Subsubsection *27.3.2.4 Estimates to a Minimizer. III* and prove (again, leaving details to the reader)

Proposition 3.6 [17]**.** *In our framework*

$$|A| \le C\kappa\ell^{-2}, \qquad |\partial A| \le C\kappa\ell^{-3} \tag{3.10}$$

and

$$|\partial A(x) - \partial A(y)| \le C_\theta\kappa\ell^{-3-\theta}|x-y|^\theta \qquad \text{as } |x-y| \le \frac{1}{2}\ell(x) \tag{3.11}$$

if $\ell(x) \ge 1$ *(for all* $\theta \in (0,1)$*).*

---

[16] Cf. Proposition 27.3.7(i).

[17] Cf. Proposition 27.3.9.

3.2 Trace Estimates

Next we can go after trace asymptotics. Recall that we are dealing with the rescaled operator. Let a be the minimal distance between nuclei (after rescaling), capped by 1; recall that $a \ge \ell_*$.

After we estimated A for $\ell(x) \lesssim 1$ in Proposition 3.1 and $e(x,x,\lambda)$ for $\ell(x) \lesssim \ell_* = h^{-2}$, we can apply arguments of Subsection 27.3.3 and arrive to

Proposition 3.7 [18]**.** *In our framework let ψ be a-admissible and supported in $\frac{1}{2}a$-vicinity of y_m, let φ be ℓ_*-admissible, supported in $2\ell_*$-vicinity and equal 1 in ℓ_*-vicinity of y_m, and let $V^0 = Z_m|x|^{-1}$. Then*

$$\mathsf{Tr}\bigl(\psi(H^-_{A,V} - H^-_{A,V^0})\psi\bigr) = \int \bigl(\mathsf{Weyl}_1(x) - \mathsf{Weyl}^0_1(x)\bigr)(1-\varphi(x))\, dx + O\bigl(a^{-\frac{1}{3}}h^{-\frac{4}{3}}\bigr). \tag{3.12}$$

Remark 3.8. Here and in Proposition 3.9 Weyl and Weyl_1 are defined for the relativistic operator (i.e. $\mathsf{Weyl} = P^{\mathsf{RTF}\prime}(V)$ and $\mathsf{Weyl} = -P^{\mathsf{RTF}}(V)$), but following arguments of 3.6 of [Ivr2], we can replace it by those for non-relativistic operator (i.e. $\mathsf{Weyl} = P^{\mathsf{TF}\prime}(V)$ and $\mathsf{Weyl} = -P^{\mathsf{TF}}(V)$) and then skip the factor $(1-\varphi(x))$.

Moreover, applying arguments of Subsection 27.3.4 we arrive to

Proposition 3.9 [19]**.** *(i) In the framework of Proposition 3.7*

$$\mathsf{Tr}\bigl(\psi(H^-_{A,V} - H^-_{A,V^0})\psi\bigr) = \int \bigl(\mathsf{Weyl}_1(x) - \mathsf{Weyl}^0_1(x)\bigr)\,\psi^2(x)(1-\varphi(x))\, dx + O\bigl(h^{-\frac{4}{3}}a^{-\frac{1}{3}}\kappa|\log\kappa|^{\frac{1}{3}} + h^{-1}a^{-\frac{1}{2}}\bigr). \tag{3.13}$$

(ii) In particular, if

$$\kappa \le ca^{-\frac{1}{6}}h^{\frac{1}{3}}|\log ah^{-2}|^{-\frac{1}{3}}, \tag{3.14}$$

then the error in (3.13) *does not exceed $Ch^{-1}a^{-\frac{1}{2}}$ exactly as in the case without magnetic field.*

---

[18] Cf. Proposition 27.3.11.
[19] Cf. Proposition 27.3.16.

Next consider the case of exactly Coulomb potential $V = Z|x|^{-1}$ and $\nu = 0$. Then

Proposition 3.10[20]**.** *Let $V = Z|x|^{-1}$, $h > 0$, $Z > 0$, and (1.8) and (1.11) be fulfilled. Then*

(i) The following limit exists[21]

$$\lim_{r\to\infty}\Bigl(\inf_A\Bigl(\operatorname{Tr}\bigl((\phi_r H_{A,V}\phi_r)^-\bigr) + \frac{1}{\kappa h^2}\int |\partial A|^2\,dx\Bigr) - \int \mathsf{Weyl}_1(x)\phi_r^2(x)\,dx\Bigr) =: 2Z^2h^{-2}S(Z\kappa, Z\beta). \tag{3.15}$$

(ii) And it coincides with (27.3.72) and also with (27.3.73).

(iii) We also can replace in Statement (i) $\operatorname{Tr}\bigl((\phi_r H_{A,V}\phi_r)^-\bigr)$ by $\operatorname{Tr}\bigl(\phi_r H^-_{A,V}\phi_r\bigr)$.

Here $\phi\in\mathscr{C}_0^\infty(B(0,1))$, $\phi = 1$ in $B(0,\frac{1}{2})$, $\phi_r = \phi(x/r)$ and Weyl and Weyl_1 are defined for non-relativistic operator.

Then we also arrive to

Proposition 3.11[22]**.** *In the framework of Proposition 3.10 for $0 < \kappa < \kappa'$, $\beta < \beta'$*

$$S(\kappa',\beta) \le S(\kappa,\beta) \le S(\kappa',\beta) + C\kappa'(\kappa^{-1} - \kappa'^{-1}), \tag{3.16}$$

$$S(\kappa,\beta) \le S(\kappa',\beta'). \tag{3.17}$$

Then, in the "atomic" case $M = 1$ we arrive instantly to the following theorem:

Theorem 3.12[23]**.** *Let $M = 1$ and (1.8) and (1.11) be fulfilled. Then*

(i) The following asymptotics holds

$$\mathsf{E}^* = \int \mathsf{Weyl}_1(x)\,dx + 2z^2S(z\kappa, z\beta)h^{-2} + O(h^{-\frac{4}{3}}\kappa|\log\kappa|^{\frac{1}{3}} + h^{-1}). \tag{3.18}$$

[20] Cf. Proposition 27.3.18.
[21] Cf. (27.3.71) and (3.18) of [Ivr2].
[22] Cf. Proposition 27.3.20 and Remark 3.8 of [Ivr2].
[23] Cf. Theorem 27.3.22 and Propositions 3.9 and 3.10 of [Ivr2].

(ii) If $\kappa = o(h^{\frac{1}{3}}|\log h|^{-\frac{1}{3}})$, *then*

$$\mathsf{E}^* = \int \mathsf{Weyl}_1^*(x)\,dx + 2z^2 S(z\kappa, z\beta)h^{-2} + o(h^{-1}), \tag{3.19}$$

in which case Weyl_1^* *must in addition to* $-h^{-3}P^{\mathsf{TF}}(W+\nu)$ *contain the Schwinger correction, and also the relativistic correction.*

Next, using arguments Subsection 27.3.6, in particular, decoupling of singularities (which is needed only in the case ofthe self-generated magnetic field), we arrive to

Theorem 3.13 [24]**.** *Let* $M \ge 2$, $\kappa \le \kappa^*$ *and* (1.8) *and* (1.11) *be fulfilled. Then*

(i) The following asymptotics holds

$$\mathsf{E}^* = \int \mathsf{Weyl}_1(x)\,dx + 2\sum_{1\le m\le M} z_m^2 S(z_m\kappa, z_m\beta)h^{-2} + O(R_1 + R_2) \tag{3.20}$$

with

$$R_1 = \begin{cases} h^{-1} + \kappa|\log\kappa|^{\frac{1}{3}}h^{-\frac{4}{3}} & \textit{if } a \ge 1,\\ a^{-\frac{1}{2}}h^{-1} + \kappa|\log\kappa|^{\frac{1}{3}}a^{-\frac{1}{3}}h^{-\frac{4}{3}} & \textit{if } h^2 \le a \le 1 \end{cases} \tag{3.21}$$

(3.22)

and

$$R_2 = \kappa h^{-2}\begin{cases} a^{-3} & \textit{if } a \ge |\log h|^{\frac{1}{3}},\\ |\log h^2 a^{-1}|^{-1} & \textit{if } h^2 \le a \le |\log h|^{\frac{1}{3}}. \end{cases} \tag{3.23}$$

(ii) If $\kappa = o(h^{\frac{1}{3}}|\log h|^{-\frac{1}{3}})$, $\kappa a^{-3} = o(h)$ *and* $a^{-1} = o(1)$, *then*

$$\mathsf{E}^* = \int \mathsf{Weyl}_1^*(x)\,dx + 2\sum_{1\le m\le M} z_m^2 S(z_m\kappa, z_m\beta)h^{-2} + o(h^{-1}). \tag{3.24}$$

---

[24] Cf. Theorem 27.3.24.

4 Main Results

4.1 Asymptotics of the Ground State Energy

Now we can apply arguments of Section 27.4. In addition to (1.8) and (1.11) we assume that

$$d := \min_{1\le m<m'\le M} |\mathsf{y}_m - \mathsf{y}_{m'}| \ge Z^{-1}, \tag{4.1}$$

$$N \asymp Z_1 \asymp \ldots \asymp Z_M. \tag{4.2}$$

Then the estimates from below follow immediately from the trace asymptotics, while for the estimate from above we need also estimate N and miscellaneous D-terems. We leave all the details to the reader.

Theorem 4.1[25]**.** *(i) Under assumptions* (1.8), (1.11), (4.1) *and* (4.2) *the following asymptotics holds*

$$\mathsf{E}^*_N = \mathcal{E}^{\mathsf{TF}}_N + \sum_{1\le m\le M} 2Z_m^2 S(\alpha Z_m, \beta Z_m) + O\bigl(Z^{\frac{4}{3}}(R_1+R_2)\bigr) \tag{4.3}$$

with R_1 *and* R_2 *defined by* (3.21) *and* (3.23) *respectively with* $\kappa = \alpha Z$, $h = Z^{-\frac{1}{3}}$ *and* $a = Z^{\frac{1}{3}}d$, d *is defined by* (4.1), $d=\infty$ *for* $M=1$.

(ii) In particular, under assumption $d \gtrsim Z^{-\frac{1}{3}}$ *the following asymptotics holds*

$$\mathsf{E}^*_N = \mathcal{E}^{\mathsf{TF}}_N + \sum_{1\le m\le M} 2Z_m^2 S(\alpha Z_m, \beta Z_m) + O\bigl(\alpha |\log(\alpha Z)|^{\frac{1}{3}} Z^{\frac{25}{9}} + Z^{\frac{5}{3}} + \alpha d^{-3} Z^2\bigr). \tag{4.4}$$

Theorem 4.2[26]**.** *(i) Let assumptions* (1.8), (1.11), (4.1) *and* (4.2) *be fulfilled and let* $\Psi = \Psi_{\boldsymbol{A}}$ *be a ground state for a near optimizer* $\boldsymbol{A}$ *of the original multiparticle problem. Then*

$$\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}}, \rho_\Psi - \rho^{\mathsf{TF}}) \le CZ^{\frac{5}{3}}. \tag{4.5}$$

[25] Cf. Theorem 27.4.3.
[26] Cf. Theorem 27.4.4.

(ii) Furthermore, if $\mathsf{d} \geq Z^{-\frac{1}{3}}$, *then*

$$\mathsf{D}(\rho_\Psi - \rho^{\mathsf{TF}}, \rho_\Psi - \rho^{\mathsf{TF}}) \leq CZ^{\frac{5}{3}}\bigl(Z^{-\delta} + (\mathsf{d}Z^{\frac{1}{3}})^{-\delta} + (\alpha Z)^{\delta}\bigr). \tag{4.6}$$

Theorem 4.3 [27]**.** *Let assumptions* (1.8), (1.11), (4.1) *and* (4.2) *be fulfilled, and let* $\alpha \leq Z^{-\frac{10}{9}}|\log Z|^{-\frac{1}{3}}$. *Then*

$$\begin{aligned}\mathsf{E}^*_N = \mathcal{E}^{\mathsf{TF}}_N + \sum_{1\leq m\leq M} 2Z_m^2 S(\alpha Z_m, \beta Z_m) + \mathsf{Dirac} + \mathsf{Schwinger} + \mathsf{RCT} +\\ O\bigl(\alpha|\log(\alpha Z)|^{\frac{1}{3}} Z^{\frac{25}{9}} + Z^{\frac{5}{3}-\delta} + \alpha \mathsf{d}^{-3} Z^2\bigr)\end{aligned} \tag{4.7}$$

where Dirac *and* Schwinger *are* Dirac *and* Schwinger correction terms *defined exactly as in non-magnetic non-relativistic case by* (25.1.29) *and* (25.1.30) *respectively, and* RCT *is relativistic correction term, defined as in the non-magnetic case by* (3.23) *of [Ivr2].*

Theorem 4.4 [28]**.** *Let assumptions* (1.8), (1.11) *and* (4.2) *be fulfilled. Let us consider* $\mathsf{y}_m = \mathsf{y}^*_m$ *minimizing the full energy*

$$\widehat{\mathsf{E}}^*_N := \mathsf{E}^*_N + \sum_{1\leq m< m'\leq M} Z_m Z_{m'} |\mathsf{y}_m - \mathsf{y}_{m'}|^{-1}. \tag{4.8}$$

Then

$$\mathsf{d} \geq \min\bigl(Z^{-\frac{5}{21}+\delta},\, Z^{-\frac{5}{21}}(\alpha Z)^{-\delta},\, \alpha^{-\frac{1}{4}} Z^{-\frac{1}{2}}\bigr) \tag{4.9}$$

and in the remainder estimates in (4.4) *and* (4.7) *one can skip* d*-connected terms; so we arrive to*

$$\mathsf{E}^*_N = \mathcal{E}^{\mathsf{TF}}_N + \sum_{1\leq m\leq M} 2Z_m^2 S(\alpha Z_m, \beta Z_m) + O\bigl(\alpha|\log(\alpha Z)|^{\frac{1}{3}} Z^{\frac{25}{9}} + Z^{\frac{5}{3}}\bigr) \tag{4.10}$$

and

$$\begin{aligned}\mathsf{E}^*_N = \mathcal{E}^{\mathsf{TF}}_N + \sum_{1\leq m\leq M} 2Z_m^2 S(\alpha Z_m) + \mathsf{Dirac} + \mathsf{Schwinger} + \mathsf{RCT} +\\ O\bigl(\alpha|\log(\alpha Z)|^{\frac{1}{3}} Z^{\frac{25}{9}} + Z^{\frac{5}{3}-\delta}\bigr)\end{aligned} \tag{4.11}$$

respectively and also the same asymptotics with $\widehat{\mathsf{E}}^*_N$ *and* $\widehat{\mathcal{E}}^{\mathsf{TF}}_N$ *instead of* E^*_N *and* $\mathcal{E}^{\mathsf{TF}}_N$.

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[27] Cf. Theorem 27.4.5.
[28] Cf. Theorem 27.4.6.

4.2 Related Problems

After Theorems 4.1–4.4 are proven, we can apply arguments of Sections 25.5 and 25.6.

Theorem 4.5 [29]**.** *Let assumptions* (1.8), (1.11) *and* (4.2) *be fulfilled.*

(i) In the framework of the fixed nuclei model let us assume that $\mathsf{I}^*_N := \mathsf{E}^*_{N-1} - \mathsf{E}^*_N > 0$*. Then*

$$(N-Z)_+ \le CZ^{\frac{5}{7}} \begin{cases} 1 & \textit{if } \ d \le Z^{-\frac{1}{3}}, \\ Z^{-\delta} + (dZ^{\frac{1}{3}})^{-\delta} + (\alpha Z)^{\delta} & \textit{if } \ d \ge Z^{-\frac{1}{3}}. \end{cases} \tag{4.12}$$

(ii) In particular, for a single atom and for molecule with $d \ge Z^{-\frac{1}{3}+\delta}$

$$(N-Z)_+ \le Z^{\frac{5}{7}}\bigl(Z^{-\delta} + (\alpha Z)^{\delta}\bigr). \tag{4.13}$$

(iii) In the framework of the free nuclei model let us assume that $\widehat{\mathsf{I}}^*_N := \widehat{\mathsf{E}}^*_{N-1} - \widehat{\mathsf{E}}^*_N > 0$*. Then estimate* (4.13) *holds.*

Theorem 4.6 [30]**.** *Let assumptions* (1.8), (1.11) *and* (4.2) *be fulfilled and let* $N \ge Z - C_0 Z^{\frac{5}{7}}$*. Then*

(i) In the framework of the fixed nuclei model

$$\mathsf{I}^*_N \le CZ^{\frac{20}{21}}. \tag{4.14}$$

(ii) In the framework of the free nuclei model with $N \ge Z - C_0 Z^{\frac{5}{7}}\bigl(Z^{-\delta} + \alpha Z^{\delta}\bigr)$

$$\widehat{\mathsf{I}}^*_N := \widehat{\mathsf{E}}^*_{N-1} - \widehat{\mathsf{E}}^*_{N-1} \le Z^{\frac{20}{21}}\bigl(Z^{-\delta'} + (\alpha Z)^{\delta'}\bigr). \tag{4.15}$$

Theorem 4.7 [31]**.** *Let assumptions* (1.8), (1.11) *and* (4.2) *be fulfilled and let* $N \le Z - C_0 Z^{\frac{5}{7}}$*. Then in the framework of the fixed nuclei model under assumption* $b \ge C_1 (N-Z)^{-\frac{1}{3}}$

$$(\mathsf{I}^*_N + \nu)_+ \le C(Z-N)^{\frac{17}{18}} Z^{\frac{5}{18}} \begin{cases} 1 & \textit{if } \ d \le Z^{-\frac{1}{3}}, \\ Z^{-\delta} + (dZ^{\frac{1}{3}})^{-\delta} & \textit{if } \ d \ge Z^{-\frac{1}{3}}. \end{cases} \tag{4.16}$$

[29] Cf. Theorem 27.5.1.

[30] Cf. Theorem 27.5.2.

[31] Cf. Theorem 27.5.3.

Theorem 4.8 [32]**.** *Let assumptions* (1.8), (1.11). *Then in the framework of free nuclei model with $M \geq 2$ the stable molecule does not exist unless*

$$Z - N \leq Z^{\frac{5}{7}}\bigl(Z^{-\delta} + (\alpha Z)^{\delta}\bigr). \tag{4.17}$$

A Some Inequalities

In this section we reproduce from [EFS2]: two new Lieb-Thirring type inequalities for the relativistic kinetic energy with a magnetic field.

Theorem A.1 [33]**.** *There exists a universal constant $C > 0$ such that for any positive number $\gamma > 0$, for any potential V with $V_+ \in \mathscr{L}^{5/2} \cap \mathscr{L}^4(\mathbb{R}^3)$, and magnetic field $B = \nabla \times A \in \mathscr{L}^2(\mathbb{R}^3)$, we have*

$$\begin{aligned}\operatorname{Tr}\Bigl(\bigl(\sqrt{\gamma^{-2}(D-A)\cdot\boldsymbol{\sigma})^2 + \gamma^{-4}} - \gamma^{-2} - U(x)\bigr)^{-}\Bigr) \geq \\ -C\Bigl\{\int U_+^{5/2}\,dx + \gamma^3 \int U_+^4\,dx + \Bigl(\int |\nabla \times A|^2\,dx\Bigr)^{3/4}\Bigl(\int U_+^4\,dx\Bigr)^{1/4}\Bigr\}.\end{aligned} \tag{A.1}$$

Notice that Theorem A.1 reduces to the well-known Daubechies inequality in the case $A = 0$ [Dau].

For the Schrödinger case, the Daubechies inequality was generalized (and improved to incorporate a critical Coulomb singularity) to non-zero A in [FLS] by using diamagnetic techniques. Theorem A.1 is the generalization of the Daubechies inequality for the Pauli operator, in which case there is no diamagnetic inequality. Moreover, in the $\gamma \to 0$ limit, (A.1) converges to the magnetic Lieb-Thirring inequality for the Pauli operator [LLS] since

$$\sqrt{\gamma^{-2}(D-A)\cdot\boldsymbol{\sigma})^2 + \gamma^{-4}} - \gamma^{-2} \to \frac{1}{2}(D-A)\cdot\boldsymbol{\sigma})^2, \qquad \gamma \to 0. \tag{A.2}$$

Theorem A.1 does not cover the case of a Coulomb singularity. The next result shows that for γ smaller than the critical value $2/\pi$, the Coulomb singularity can be included.

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32) Cf. Theorem 27.5.6.

33) Theorem 2.2 of [EFS2].

34) Theorem 2.3 of [EFS2].

Theorem A.2 [34]**.** *Let* ϕ_r *be a real function satisfying* $\operatorname{supp}\phi_r \subset \{|x| \le r\}$, $\|\phi_r\|_\infty \le 1$. *There exists a constant* $C > 0$ *such that if* $\gamma \in (0, 2/\pi)$, *then*

$$\operatorname{Tr}\Big(\phi_r\big(\sqrt{\gamma^{-2}(D-A)\cdot\boldsymbol{\sigma})^2+\gamma^{-4}} - \gamma^{-2} - \frac{1}{|x|} - U\big)\phi_r\Big)^- \tag{A.3}$$
$$\ge -C\Big\{\eta^{-3/2}\int |\nabla\times A|^2\,dx + \eta^{-3}r^3 + \eta^{-3/2}\int U_+^{5/2}\,dx + \eta^{-3}\gamma^3\int U_+^4\,dx$$
$$+ \Big(\int |\nabla\times A|^2\,dx\Big)^{3/4}\Big(\int U_+^4\,dx\Big)^{1/4}\Big\},$$

where $\eta := \frac{1}{10}(1-(\pi\gamma/2)^2)$.

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Complete Semiclassical Spectral Asymptotics for Periodic and Almost Periodic Perturbations of Constant Operators*,†

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Abstract

Under certain assumptions we derive a complete semiclassical asymptotics of the spectral function $e_{h,\varepsilon}(x,x,\lambda)$ for a scalar operator

$$A_\varepsilon(x,hD) = A^0(hD) + \varepsilon B(x,hD),$$

where A^0 is an elliptic operator and $B(x,hD)$ is a periodic or almost periodic perturbation.

In particular, a complete semiclassical asymptotics of the integrated density of states also holds. Further, we consider generalizations.

1 Introduction

1.1 Preliminary Remarks

This work is inspired by several remarkable papers of L. Parnovski and R. Shterenberg [PS1,PS2,PS3], S. Morozov, L. Parnovski and R. Shterenberg [MPS] and earlier papers by A. Sobolev [So1,So2]. I wanted to understand the approach of the authors and, combining their ideas with my own approach, generalize their results.

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In these papers the complete asymptotic expansion of the integrated density of states $\mathsf{N}(\lambda)$ for operators $\Delta+V$ was derived as $\lambda\to+\infty$; here Δ is a positive Laplacian and V is a periodic or almost periodic potential (satisfying certain conditions). In [MPS] more general operators were considered.

Further, in [PS3] the complete asymptotic expansion of $e(x,x,\lambda)$ was derived, where $e(x,y,\lambda)$ is the Schwartz kernel of the spectral projector.

I borrowed from these papers Conditions 1.2–1.6 and the *special gauge transformation* and added the *hyperbolic operator method* (actually non-stationary semiclassical Schrödinger operator method– [Ivr1]) and extremely long propagation of singularities. I believe that this is a simpler and more powerful approach. Also, in contrast to those papers I consider more general semiclassical asymptotics.

Consider a scalar self-adjoint h-pseudo-differential operator $A(x,hD)$ in $\mathbb{R}^d$ with the Weyl symbol $A(x,\xi)$, such that

$$|D_x^\alpha D_\xi^\beta A(x,\xi)|\le c_{\alpha\beta}(|\xi|+1)^m\qquad\forall\alpha,\beta\ \forall x,\xi \tag{1.1}$$

and

$$A(x,\xi)\ge c_0|\xi|^m-C_0\qquad\forall x,\xi. \tag{1.2}$$

Then it is semibounded from below. Let $e_h(x,y,\lambda)$ be the Schwartz kernel of its spectral projector $E(\lambda)=\theta(\lambda-A)$. We are interested in the semiclassical asymptotics of $e_h(x,x,\lambda)$ and

$$\mathsf{N}_h(\lambda)=\mathsf{M}[e(x,x,\lambda)]\ :=\lim_{\ell\to\infty}(\mathsf{mes}(\ell X))^{-1}\int_{\ell X}e(x,x,\lambda)\,dx, \tag{1.3}$$

where $0\in X$ is an open domain in $\mathbb{R}^d$. The latter expression in the cases we are interested in does not depend on X and is called *Integrated Density of States*.

It is well-known that under *ξ-microhyperbolicity condition on the energy level λ*

$$|A(x,\xi,h)-\lambda|+|\nabla_\xi A(x,\xi,h)|\ge\epsilon_0 \tag{1.4}$$

the following asymptotics holds

$$e_h(x,x,\lambda)=\kappa_0(x,\lambda)h^{-d}+O(h^{1-d})\qquad\text{as}\ \ h\to+0, \tag{1.5}$$

and therefore

$$\mathsf{N}_h(\lambda)=\bar\kappa_0(\lambda)h^{-d}+O(h^{1-d}), \tag{1.6}$$

where here and below

$$\bar{\kappa}_n(\lambda) = \mathsf{M}[\kappa_n(x,\lambda)]. \tag{1.7}$$

For generalization to matrix operators and degenerate scalar operators see Chapters 4 and 5 respectively. Also there one can find slightly sharper two-term asymptotics under non-periodicity conditions.

Also it is known (see Chapter 4) that under microhyperbolicity condition (1.4) for $|\tau-\lambda|<\epsilon$ the following complete asymptotics holds:

$$F_{t\to h^{-1}\tau}\bigl(\bar{\chi}_T(t)\bigl(Q_{2x}u_h(x,y,t)\,{}^tQ_{1y}\bigr)|_{y=x}\bigr) \sim \sum_{n\ge 0}\kappa'_{n,Q_1,Q_2}(x,\tau)h^{1-d+n}, \tag{1.8}$$

where $u_h(x,y,t)$ is the Schwartz kernel of of the *propagator* $e^{ih^{-1}tA}$, $\bar{\chi}\in\mathscr{C}_0^\infty([-1,1])$, $\bar{\chi}(t)=1$ at $[-\frac{1}{2},\frac{1}{2}]$, $T\in[h^{1-\delta},T^*]$, T^* is a small constant here and $Q_j=Q_j(x,hD)$ are h-pseudo-differential operator; we write operators, acting with respect to y on Schwartz kernels to the right of it.

Further, it is known that

$$\mathsf{supp}(Q_1)\cap\mathsf{supp}(Q_2)=\emptyset \implies \kappa'_{n,Q_1,Q_2}(x,\tau)=0, \tag{1.9}$$

where $\mathsf{supp}(Q_j)$ is a support of its symbol $Q_j(x,\xi)$ and

$$\tau\le\tau^*=\inf_{x,\xi}A(x,\xi) \implies \kappa'_{n,Q_1,Q_2}(x,\tau)=0. \tag{1.10}$$

Let

$$\kappa_{n,Q_1,Q_2}(x,\tau)=\int_{-\infty}^{\tau}\kappa'_{n,Q_1,Q_2}(x,\tau')\,d\tau. \tag{1.11}$$

In what follows we skip subscripts $Q_j=I$.

Remark 1.1. This equality (1.8) plus Hörmander's Tauberian theorem imply the remainder estimates $O(h^{1-d})$ for $Q_{2x}e_h(x,y,\tau)\,{}^tQ_{1y}|_{x=y}$. On the other hand, if we can improve (1.8) by increasing T^*, we can improve the remainder estimate to $O(T^{*\,-1}h^{1-d})$ [1),2)].

Observe that for $A=A(hD)$

$$e_h(x,x,\lambda)=\mathsf{N}_h(\lambda)=\kappa_0(\lambda)h^{-d}. \tag{1.12}$$

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1) Provided $T^*=O(h^{-M})$ for some M.

2) This plus estimate for κ'_0 is a major method for obtaining sharp remainder estimates in [Ivr1].

In this paper we consider

$$A(x,hD)=A^0(hD)+\varepsilon B(x,hD), \tag{1.13}$$

where $A^0(\xi)$ satisfies (1.1), (1.2) and (1.4) and $B(x,\xi)$ satisfies (1.1) and $\varepsilon>0$ is a small parameter. Later we assume that $B(x,hD)$ is almost periodic and impose other conditions.

First, we claim that for operator (1.13) with $\varepsilon\le\epsilon_0$ the equality (1.8) holds with $T^*=\epsilon_1\varepsilon^{-1}$ where ϵ_j are small constants and we assume that $\varepsilon\ge h^M$ for some M. Then the remainder estimate is $O(\varepsilon h^{1-d})$ [3)].

1.2 Main Theorem

Now we consider the main topic of this work where we will use ideas from [PS1,PS2,PS3,MPS]: the case of an almost periodic operator $B(x,hD)$,

$$B(x,\xi)=\sum_{\theta\in\Theta} b_\theta(\xi)e^{i\langle\theta,x\rangle} \tag{1.14}$$

with discrete (i.e. without any accumulation points) *frequency set* Θ.

Operator B is *quasiperiodic* if Θ is a finite set, *periodic* if Θ is a lattice and *almost periodic* in the general case.

Our goal is to derive (under certain assumptions) complete semiclassical asymptotics:

$$e_{h,\varepsilon}(x,x,\tau)\sim\sum_{n\ge 0}\kappa_{n,\varepsilon}x(x,\tau)h^{-d+n}. \tag{1.15}$$

First, in addition to microhyperbolicity condition (1.4) we assume that $\Sigma_\lambda=\{\xi\colon A^0(\xi)=\lambda\}$ is a *strongly convex surface* i.e.

$$\pm\sum_{j,k}A^0_{\xi_j\xi_k}(\xi)\eta_j\eta_k\ge\epsilon|\eta|^2 \qquad \forall\xi\colon A^0(\xi)=\lambda\ \ \forall\eta\colon \sum_j A^0_{\xi_j}(\xi)\eta_j=0, \tag{1.16}$$

where the sign depends on the connected component of Σ_λ, containing ξ.

Without any loss of generality we assume that

(1.17) Θ spans $\mathbb{R}^d$, contains 0 and is symmetric about 0.

[3)] See Theorem 2.4.

Condition 1.2. *For each* $\theta_1,\dots,\theta_d\in\Theta$ *<u>either</u>* $\theta_1,\dots,\theta_d$ *are linearly independent over* $\mathbb{R}$ *<u>or</u> they linearly dependent over* $\mathbb{Z}$.

Assume also that

Condition 1.3. *For any arbitrarily large* L *and for any sufficiently large real number* ω *there are a finite symmetric about* 0 *set* $\Theta':=\Theta'_{(L,\omega)}\subset(\Theta\cap\mathsf{B}(0,\omega))$ *(with* $\mathsf{B}(\xi,r)$ *the ball of the radius* r *and center* ξ*) and a "cut-off" coefficients* $b'_\theta:=b'_{\theta,(L,\omega)}$, *such that*

$$B':=B'_{(L,\omega)}(x,\xi):=\sum_{\theta\in\Theta'}b'_\theta(\xi)e^{i\langle\theta,x\rangle}\tag{1.18}$$

satisfies

$$\|D_x^\alpha D_\xi^\beta\bigl(B-B'\bigr)\|_{\mathscr{L}^\infty}\le\omega^{-L}(|\xi|+1)^m\qquad\forall\alpha,\beta\colon|\alpha|\le L,|\beta|\le L.\tag{1.19}$$

Remark 1.4. (i) Then

$$|D_\xi^\beta b_\theta|=O(|\theta|^{-\infty}(|\xi|+1)^m)\qquad\text{as}\quad|\theta|\to\infty\tag{1.20}$$

and

$$|D_\xi^\beta(b_\theta-b'_\theta)|=O(\omega^{-\infty}(|\xi|+1)^m).\tag{1.21}$$

Indeed, one suffices to observe that $b_\theta(\xi)=\mathsf{M}(B(x,\xi)e^{-i\langle\theta,x\rangle})$ etc.

(ii) On the other hand, under additional assumption

$$\#\{\theta\in\Theta,\ |\theta|\le\omega\}=O(\omega^p)\qquad\text{as}\quad\omega\to\infty\tag{1.22}$$

for some p, (1.20) implies Condition 1.3 with $\Theta'_{(L,\omega)}:=\Theta\cap\mathsf{B}(0,\omega)$. However we will need $\Theta'_{(L,\omega)}$ in the next condition.

(iii) We need only to estimate the operator norm of the difference between $B(x,hD)$ and $B'(x,hD)$ (from $\mathscr{H}^m$ to $\mathscr{L}^2$); therefore for differential operators we can weaken (1.19): if

$$B=\sum_{\mu,\nu:|\alpha|\le m',|\beta|\le m'}D^\alpha b_{\alpha\beta}(x)D^\beta,\qquad b_{\alpha\beta}=b^\dagger_{\beta\alpha},\tag{1.23}$$

where we assume that $b_{\alpha\nu}(x)$ and $b'_{\alpha\beta}(x)$ have similar decompositions (1.14) and (1.18) respectively, then (1.19) should be replaced by

$$\|D_x^\alpha\bigl(b_{\alpha\beta}-b'_{\alpha\beta}\bigr)\|_{\mathscr{L}^\infty}\le\omega^{-L}\qquad\forall\alpha.\tag{1.24}$$

(iv) While Condition 1.3 is Condition B of [PS3], adopted to our case, Condition 1.2 and Conditions 1.5, 1.6 below are borrowed without any modifications (except changing notations).

The next condition we need to impose is a version of the Diophantine condition on the frequencies of B. First, we need some definitions. We fix a natural number K (the choice of K will be determined later by how many terms in the asymptotic decomposition of $e(x,x,\lambda)$ we want to obtain) and consider Θ'_K, which here and below denotes the algebraic sum of K copies of Θ':

$$\Theta'_K := \sum_{1\le i\le K} \Theta. \tag{1.25}$$

We say that $\mathfrak{V}$ is a *quasilattice subspace* of dimension q, if $\mathfrak{V}$ is a linear span of q linear independent vectors $\theta_1, \dots, \theta_q \in \Theta'_K \setminus 0$. Obviously, the zero space is a quasilattice subspace of dimension 0 and $\mathbb{R}^d$ is a quasilattice subspace of dimension d.

We denote by $\mathcal{V}_q$ the collection of all quasilattice subspaces of dimension q and also $\mathcal{V} := \bigcup_{q\ge 0} \mathcal{V}_q$.

Consider $\mathfrak{V}, \mathfrak{U} \in \mathcal{V}$. We say that these subspaces are *strongly distinct*, if neither of them is a subspace of the other one. Next, let $\widehat{(\mathfrak{V}, \mathfrak{U})} \in [0, \pi/2]$ be the angle between them, i.e. the angle between $\mathfrak{V} \ominus \mathfrak{W}$ and $\mathfrak{U} \ominus \mathfrak{W}$, $\mathfrak{W} = \mathfrak{U} \cap \mathfrak{V}$. This angle is positive iff $\mathfrak{V}$ and $\mathfrak{U}$ are strongly distinct.

Condition 1.5. *For each fixed L and K the sets $\Theta'_{(L,\omega)}$ satisfying (1.18) and (1.19) can be chosen in such a way that for sufficiently large ω we have*

$$s(\omega) = s(\Theta'_K) := \inf_{\mathfrak{V},\mathfrak{U}\in\mathcal{V}} \sin(\widehat{(\mathfrak{V}, \mathfrak{U})}) \ge \omega^{-1} \tag{1.26}$$

and

$$r(\omega) := \inf_{\theta\in\Theta'_K\setminus 0} |\theta| \ge \omega^{-1}, \tag{1.27}$$

where the implied constant (i.e. how large should ω be) depends on L and K.

Let $\mathfrak{V}$ be the span of $\theta_1, \dots, \theta_q \in \Theta'_K \setminus 0$. Then due to Condition 1.2 each element of the set $\Theta'_K \cap \mathfrak{V}$ is a linear combination of $\theta_1, \dots, \theta_q$ with rational coefficients. Since the set $\Theta'_K \cap \mathfrak{V}$ is finite, this implies that the set $\Theta'_\infty \cap \mathfrak{V}$ is discrete and is, therefore, a lattice in $\mathfrak{V}$. We denote this lattice by $\Gamma(\omega; \mathfrak{V})$.

Our final condition states that this lattice cannot be too dense.

Condition 1.6. *We can choose $\Theta'_{(L;\omega)}$, satisfying Conditions 1.3 and 1.5 in such a way that for sufficiently large ω and for each $\mathfrak{V}\in\mathcal{V}$, $\mathfrak{V}\ne\mathbb{R}^d$, we have*

$$\operatorname{vol}(\mathfrak{V}/\Gamma(\omega;\mathfrak{V}))\ge\omega^{-1}. \tag{1.28}$$

Remark 1.7. See Section 2 of [PS3] for discussion of these conditions. In particular, if Θ is a lattice, then Conditions 1.2–1.6 are fulfilled. Further, if Θ is a finite set and Condition 1.2 is fulfilled, then $\Theta_\infty := \bigcup_{K\ge1}\Theta_K$ is a lattice and Conditions 1.3–1.6 are fulfilled. Furthermore, the same is true, if Θ is an arithmetic sum of a finite set and a lattice.

The main theorem of this paper is

Theorem 1.8. *Let A be a self-adjoint operator* (1.13)*, where A^0 satisfies* (1.1)*,* (1.2)*,* (1.4) *and* (1.16) *and B satisfies* (1.1)*.*

Let Conditions 1.2–1.6 be fulfilled. Then for $|\tau-\lambda|<\epsilon$, $\varepsilon\le h^\vartheta$, $\vartheta>0$

$$e_{h,\varepsilon}(x,x,\tau)\sim\sum_{n\ge0}\kappa_n(x,\tau;\varepsilon)h^{-d+n}. \tag{1.29}$$

Corollary 1.9. *In the framework of Theorem 1.8*

$$\mathsf{N}_{h,\varepsilon}(\tau)\sim\sum_{n\ge0}\bar\kappa_n(\tau;\varepsilon)h^{-d+n}. \tag{1.30}$$

1.3 Plan of the Paper

Section 2 is devoted to the proof of Theorem 1.8. In Subsection 2.1 we make some general remarks, and, in particular, we prove more general albeit far less precise Theorem 2.4. Then, in Subsection 2.2 we describe a gauge transformation.

In Subsection 2.3 we consider a non-resonant zone and justify such transformation, which reduces operator microlocally to a constant symbol operator $A''(hD,h)$. This allows us to study a propagation of singularities with respect to ξ and prove that the singularities do not propagate with respect to ξ [4]. In Subsection 2.5 we consider a resonant zone and justify such transformation, which reduces operator microlocally to an operator

[4] For time $T^*=h^{-M}$ with arbitrarily large M.

$A''(x', hD, h)$, where $x' \in \mathfrak{V}$ the corresponding resonant subspace, and prove that the singularities propagate only with respect to ξ'. Then the convexity condition implies that the singularities actually do not propagate with respect to ξ [4)].

In Subsection 2.6 we consider propagation with respect to x and using the results of Subsections 2.3 and 2.5 we prove that the singularities "propagate away" and do not return[4)]. The we apply Tauberian theorem with $T = T^*$ and prove Theorem 1.8.

In Section 3 we generalize Theorem 1.8. First, in Subsection 3.1 we consider matrix operators with the simple eigenvalues of $A^0(\xi)$.

Then, in Subsection 3.2 we consider operators $A^0(hD) + \varepsilon V(x, hD)$ where symbol $V(x, \xi)$ decays as $|x| \to \infty$ and hybrid operators $A^0(hD) + \varepsilon(B(x, hD) + V(x, hD))$ with almost periodic B and decaying V and show that our methods work for them as well.

Finally, in Subsection 3.3 we discuss differentiability of our asymptotics with respect to τ.

2 Proof of the Main Theorem

2.1 Preliminary Analysis

Remark 2.1. (i) It follows from Section 4 that the contribution of the zone $\{\xi \colon |A^0(\xi) - \tau| \ge C_0\varepsilon + h^{1-\varsigma}\}$ to the remainder is negligible. Here and below $\varsigma > 0$ is an arbitrarily small exponent. Namely, let $Q_j = Q_j(hD)$ be operators with the symbols $Q_j(\xi)$, such that

$$\operatorname{supp}(Q_1) \cap \operatorname{supp}(Q_2) \cap \Omega_\tau = \emptyset \tag{2.1}$$

with

$$\Omega_\tau := \{\xi \colon |A^0(\xi) - \tau| \le C_0\varepsilon + h^{1-\varsigma}\} \tag{2.2}$$

and satisfying

$$|D^\alpha Q_j| \le C_\alpha h^{-(1-\varsigma)|\alpha|} \qquad \forall \alpha. \tag{2.3}$$

Then

$$(Q_{2x} e(x, y, \tau)\, {}^t Q_{1y})|_{y=x} = \kappa_{0,Q_1,Q_2} h^{-d} + O(h^\infty) \tag{2.4}$$

with

$$\kappa_{0,Q_1,Q_2} = (2\pi)^{-d} \int \theta(\tau - A^0(\xi)) Q_1(\xi) Q_2(\xi)\, d\xi \tag{2.5}$$

with $\theta(\tau - A^0(\xi))$ equal to either 0 or 1 on each connected component of $\Omega_\tau \cap \operatorname{supp}(Q_1) \cap \operatorname{supp}(Q_2))$.

Therefore we restrict ourself by the analysis in the zone Ω_τ.

(ii) To upgrade (1.8) with $T = T_*$ (a small constant) to (1.8) with $T = T^*$ it is sufficient to prove that

$$|F_{t\to h^{-1}\tau}\bigl(\chi_T(t)\bigl(Q_{2x}u_h(x,y,t)\,{}^tQ_{1y}\bigr)\bigr|_{y=x}\bigr)| \le C_s h^{-d+s}, \tag{2.6}$$

for $|\tau - \lambda| \le \epsilon$, $T \in [T_*,\ T^*]$ and $\chi \in \mathscr{C}_0^\infty([-1,-\frac{1}{2}] \cup [\frac{1}{2},1])$, where s is an arbitrarily large exponent.

In the very general setting for $|t| \le h^{-M}$ the propagation speed with respect to ξ does not exceed $C\varepsilon$. More precisely

Proposition 2.2. *Let $A = A^0 + \varepsilon B$ where $A^0(hD)$ and $B(x,hD)$ are matrix operators satisfying* (1.1)*. Let $Q_j(hD)$ be operators with symbols satisfying* (2.3)*. Further, let $\operatorname{supp}(Q_j) \subset \{\xi\colon |\xi| \le c\}$ and*

$$\operatorname{dist}(\operatorname{supp}(Q_1),\ \operatorname{supp}(Q_2)) \ge \max(C_0\varepsilon T,\ h^{1-\varsigma}) \tag{2.7}$$

with $T \le h^{-M}$. Then for $|t| \le T$

$$\|Q_2 e^{ih^{-1}tA} Q_1\| \le C_{M,s}h^s. \tag{2.8}$$

Proof. One can prove easily by arguments of the proof of Theorem 2.1.2, applied to operator $\varepsilon^{-1}A = \varepsilon^{-1}A^0(hD_x) + B(x,hD)$ and $\phi(\xi,t)$, that the propagation speed with respect ξ does not exceed C_0; presence of the term $\varepsilon^{-1}A^0(hD_x)$ does not matter since it disappears in the commutator with $\phi(hD)$. Changing $t \mapsto \varepsilon t$ we conclude that for operator A the propagation speed with respect to ξ does not exceed $C_0\varepsilon$.

We do not need compactness of the domain in the phase space with respect to x since the propagation speed with respect to x does not exceed C_0 and we have such compactness implicitly. We leave easy details to the reader. □

Proposition 2.3. *In the framework of Proposition 2.2 assume that $A^0(hD)$ is microhyperbolic on the energy level λ* [5]*.*

Then for $T_* \le T \le T^* = \min(\epsilon_0\varepsilon^{-1}, h^{-M})$ (2.6) *holds.*

[5] For definition for matrix operators see Definition 2.1.1.

Proof. It is sufficient to prove for $\mathsf{supp}(Q_1)$ contained in the small vicinity of some point $\bar{\xi}$. Then due to Proposition 2.2 $e^{ih^{-1}tA}Q_1 \equiv Q_2 e^{ih^{-1}tA}Q_1$ modulo operators with $O(h^\infty)$-norms [6] and with Q_2 also supported in the small vicinity of $\bar{\xi}$ and equal 1 in the vicinity of $\mathsf{supp}(Q_1)$.

Then on $\mathsf{supp}(Q_2)$ operator is microhyperbolic with respect to vector ℓ and we can employ the proof of Theorem 2.1.2 again, this time with $\phi(x,t) = \ell x - \epsilon_0 t$. For further details see Chapter 4. □

Then in virtue of (1.8) with $t = T_*$ (which is also due to the microhyperbolicity condition) (1.8) also holds with $T = T^*$ and applying Hörmander's Tauberian theorem we arrive to the remainder estimate $Ch^{1-d}T^{*\,-1} = C\varepsilon h^{1-d}$, thus proving the following theorem:

Theorem 2.4. *Let $A = A^0(hD) + \varepsilon B(x, hD)$ with A^0 satisfying conditions* (1.1), (1.2) *and* (1.4) *and B satisfying conditions* (1.1). *Then*

$$e_h(x,x,\tau) = \sum_{0\le n\le M} \kappa_n(x,\tau)h^{-d+n} + O(\varepsilon h^{1-d}) \tag{2.9}$$

provided $\varepsilon \ge h^M$, $|\tau - \lambda| \le \epsilon$.

From now on we discuss only Theorem 1.8.

Remark 2.5. (i) It suffices to prove asymptotics

$$e_h(x,x,\tau) = \sum_{0\le n\le M} \kappa_n(x,\tau)h^{-d+n} + O(h^{-d+M}) \tag{2.10}$$

with arbitrarily large fixed M. To do so we will use the *hyperbolic operator method* (which we implement as *semiclassical Schrödinger operator method*) with maximal time $T^* = h^{-M}$.

(ii) Then we can replace operator B by operator B', provided operator norm of $B - B'$ from $\mathscr{H}^m$ to $\mathscr{L}^2$ does not exceed Ch^{3M}.

Indeed, let $A' = A^0 + \varepsilon B'$. Due to Remark 2.1 we need to compare only $Q_1 e^{ih^{-1}tA'}Q_1$ and $Q_1 e^{ih^{-1}tA}Q_1$. Observe that due to (1.2)

$$\| e^{ih^{-1}tA}Q_1 - Q_2 e^{ih^{-1}tA}Q_1 \|_k \le C_{k,s}h^s$$

[6] By default, operator norm is from $\mathscr{L}^2$ to $\mathscr{L}^2$.

with arbitrarily large k, s, where $|||.|||_k$ denotes an operator norms from $\mathscr{L}^2$ to $\mathscr{H}^k$ provided $\mathsf{supp}(Q_j) \subset \{\xi\colon A^0(\xi) \le 2jc\}$ and $Q_2 = 1$ in $\{\xi\colon A^0(\xi) < 3c\}$. The same is true for A' as well.

Then equality

$$e^{ih^{-1}tA'} - e^{ih^{-1}tA} = ih^{-1}\int_0^t e^{ih^{-1}(t-t')A}(A'-A)e^{ih^{-1}t'A'}\,dt'$$

and restriction $|t| \le T^*$ imply that $|||\bigl(e^{ih^{-1}tA'} - e^{ih^{-1}tA}\bigr)Q|||_k$ does not exceed $C_{k,s}h^s + Ch^{-1-M}|||Q_2(B-B')Q_2|||_k$.

Finally, observe that $|||Q_2(B-B')Q_2|||_k \le C_k h^{-k-m}|||(B-B')|||'_k$ where $|||.|||'_k$ denotes an operator norm from $\mathscr{H}^m$ to $\mathscr{L}^2$.

(iii) Since $\mathsf{N}_h(\tau)$ could be defined equivalently as

$$\mathsf{N}_h(\lambda) = \lim_{\ell\to\infty}(\mathsf{mes}(\ell X))^{-1}\mathsf{N}_h(\lambda,\ell X)e(x,x,\lambda)\,dx, \tag{2.11}$$

where $\mathsf{N}_h(\lambda, X)$ is an eigenvalue counting function for operator A in X with the Dirichlet (or Neumann–does not matter) boundary conditions on ∂X, for $\mathsf{N}_h(\tau)$ we can arrive to the same conclusion from the variational arguments.

(iv) First such replacement will be $B' := B'_{(L,\omega)}$ from Condition 1.3 with $\omega = h^{-\sigma}$, arbitrarily small $\sigma > 0$ and $L = 3M/\sigma$.

So, from now Θ and B are effectively replaced by $\Theta' := \Theta'_{(L,\omega)}$ and $B'_{(L,\omega)}$ correspondingly.

2.2 Gauge Transformation

Consider now the "gauge" transformation $A \mapsto e^{-i\varepsilon h^{-1}P}Ae^{i\varepsilon h^{-1}P}$ with h-pseudodifferential operator P. Observe that

$$\begin{aligned}e^{-i\varepsilon h^{-1}P}Ae^{i\varepsilon h^{-1}P} &= A - i\varepsilon h^{-1}[P,A] + \sum_{2\le n\le K-1}\frac{1}{n!}(-i\varepsilon h^{-1})^n\,\mathsf{Ad}_P^n(A)\\ &+ \int_0^1 \frac{1}{(K-1)!}(1-s)^{K-1}(-i\varepsilon h^{-1})^K e^{-i\varepsilon h^{-1}sP}\,\mathsf{Ad}_P^K(A)e^{i\varepsilon h^{-1}sP}\,ds,\end{aligned} \tag{2.12}$$

where $\mathsf{Ad}_P^0(A) = A$ and $\mathsf{Ad}_P^{n+1}(A) = [P, \mathsf{Ad}_P^n(A)]$ for $n = 0, 1, \dots$.

Thus *formally* we can compensate εB, taking

$$P=\sum_{\theta} ih\bigl(A^0(\xi+\theta h/2)-A^0(\xi-\theta h/2)\bigr)^{-1}b_\theta(\xi)e^{i\langle\theta,x\rangle}, \tag{2.13}$$

so that

$$ih^{-1}[P,A^0]=B \implies ih^{-1}[P,A]=B+i\varepsilon h^{-1}[P,B]. \tag{2.14}$$

Then perturbation εB is replaced by $\varepsilon^2 B'$, which is the right hand expression in (2.12) minus A^0, i.e.

$$B'=-ih^{-1}[P,B]+\sum_{2\le n\le K-1}\frac{1}{n!}\varepsilon^{n-2}(-ih^{-1})^n\operatorname{Ad}_P^n(A), \tag{2.15}$$

where we ignored the remainder.

New perturbation, again formally, has a magnitude of ε^2. Repeating this process we will make a perturbation negligible.

Remark 2.6. However, we need to address the following issues issues:

(i) Denominator $h^{-1}\bigl(A^0(\xi+\theta h/2)-A^0(\xi-\theta h/2)\bigr)=\langle\nabla_\xi A^0,\theta\rangle+O(h^{1-\sigma})$ could be small.

(ii) In B' set Θ' increases: $\varepsilon^2B'=\varepsilon^2B'_2+\varepsilon^3B'_3+\ldots+\varepsilon^MB'_M$, where for B'_j the frequency set is Θ'_j (the arithmetic sum of j copies of Θ').

(iii) We need to prove that the remainder is negligible.

(iv) This transformation was used in Section 9 of [PS3] (etc); in contrast to these papers we use Weyl quantization instead of pq-quantization, and have therefore $\bigl(A^0(\xi+\theta h/2)-A^0(\xi-\theta h/2)\bigr)$ instead of $\bigl(A^0(\xi+\theta h)-A^0(\xi)\bigr)$.

2.3 Non-Resonant Zone

2.4 Gauge Transformation

One can see easily that if inequality

$$|\langle\nabla_\xi A^0(\xi),\theta\rangle|\ge\gamma:=\varepsilon^{\frac12}h^{-\delta} \tag{2.16}$$

holds for all $\theta \in \Theta'_K \setminus 0$, then the terms could be estimated by $h^{\delta n}$ and our construction works with $K = 3M/\delta$. Here and below without any loss of the generality we assume that $\varepsilon \geq h$; so, in fact,

$$h^{\vartheta} \geq \varepsilon \geq h. \tag{2.17}$$

Indeed, if $P = P(x, hD)$ has the symbol, satisfying

$$|D_\xi^\alpha D_x^\beta P| \leq c_{\alpha\beta}\gamma^{-1-|\alpha|} \qquad \forall \alpha, \beta, \tag{2.18}$$

then $B' = \varepsilon h^{-1}[P, B]$ has a symbol, satisfying

$$|D_\xi^\alpha D_x^\beta B'| \leq c'_{\alpha\beta}\varepsilon\gamma^{-2-|\alpha|} \qquad \forall \alpha, \beta, \tag{2.19}$$

so indeed $\varepsilon' = \varepsilon\gamma^{-2}$.

Then we can eliminate a perturbation completely, save terms with the frequency 0, both old and new. The set of ξ satisfying (2.16) for all $\theta \in \Theta'_K$ we call *non-resonant zone* and denote by $\mathcal{Z}$. Thus, we arrive to

Proposition 2.7. *Let $Q = Q(hD)$ with the symbol supported in $\mathcal{Z} \cap \Omega$ and satisfying* (2.3)

Then there exists a pseudo-differential operator $P = P(x, hD)$ with the symbol, satisfying (2.18) *and such that*

$$\bigl(e^{-i\varepsilon h^{-1}P} A e^{i\varepsilon h^{-1}P} - A''\bigr) Q \equiv 0 \tag{2.20}$$

with

$$A'' = A^0(hD) + \varepsilon B''_0(hD) \tag{2.21}$$

modulo operator from $\mathscr{H}^m$ to $\mathscr{L}^2$ with the operator norm $O(h^{3M})$.

Remark 2.8. (i) This proposition is similar to Lemma 9.3 of [PS3]. However, in contrast to [PS1, PS2, PS3, MPS], after it is proven we do not write asymptotic decomposition there, but simply prove that singularities do not propagate with respect to ξ there.

(ii) It is our second replacement of operator A; recall that the first one was based on Condition 1.3, and now we ignore the remainder after transformation, which is justified by Remark 2.5(i).

Propagation.

Proposition 2.9. *Let* $Q_j = Q_j(hD)$ *with the symbols, satisfying* (2.3) *and let symbol of* Q_1 *be supported in* $\mathcal{Z}\cap\Omega$.

Let $\mathsf{dist}(\mathsf{supp}(Q_1), \mathsf{supp}(Q_2)) \ge c\gamma$. *Then*

$$\|Q_2 e^{ih^{-1}tA} Q_1\| = O(h^{2M}) \qquad as \quad |t|\le T^* = h^{-M}. \tag{2.22}$$

Proof. One can prove easily that the operator norms of $Q_2 e^{ih^{-1}tA''}Q_1$ and $Q_2 e^{\pm i\varepsilon h^{-1}P}Q_1$ are $O(h^{2M})$. We leave all easy details to the reader. □

2.5 Resonant Zone

Consider now *resonant zone*

$$\Lambda := \bigcup_{\theta\in\Theta'_K\setminus 0} \Lambda(\theta), \tag{2.23}$$

where $\Lambda(\theta)$ is the set of ξ, violating (2.16) for given θ:

$$\Lambda(\theta) = \Lambda_\delta(\theta) := \{\xi\colon |\langle\nabla_\xi A^0(\xi),\theta\rangle| \ge \gamma = c\varepsilon^{\frac{1}{2}}h^{-\delta}\}. \tag{2.24}$$

Case $d = 2$. We start from the easiest case $d=2$ (in the trivial case $d=1$ there is no resonant zone). Observe that due to assumption (1.16) for each θ

$$\mathsf{mes}_1(\Lambda(\theta)\cap\Sigma_\lambda) \le C\gamma. \tag{2.25}$$

Further, $\#\Theta'_K \le Ch^{-\sigma}$ (as $h\le h_0(K,\sigma)$) due to Condition 1.5. Thus $\mathsf{mes}_1(\Lambda\cap\Sigma_\lambda)\le \gamma h^{-\sigma}$. Recall, that $\sigma>0$ is arbitrarily small.

Since due to Proposition 2.9, the propagation which starts in the non-resonant zone $\mathcal{Z}$ remains there[7)] we conclude that the propagation which is started in some connected component of the resonant zone also remains there[7)].

Thus, $\nabla_\xi A^0(\xi)$ does not change by more than $\gamma h^{-\sigma}$ and since σ ais arbitrarily small we conclude that (2.22) also holds for Q_1, supported in the resonant zone. Therefore

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[7)] May be, with different constant c in the definition of γ.

(2.26) Estimate (2.22) holds for all Q_1, Q_2 satisfying (2.3) and

$$\mathsf{dist}(\mathsf{supp}(Q_1), \mathsf{supp}(Q_2)) \geq \gamma. \tag{2.27}$$

Remark 2.10. (i) In the proof of Theorem 1.8 we need only to have estimate (2.22) holding for all Q_1, Q_2 satisfying (2.3) and (2.27) with arbitrarily small constant γ.

(ii) Then for $d = 2$ we can replace assumption (1.16) by

(2.28) $\varkappa(s)$ (a curvature of Σ_λ, naturally parametrized by s) has zeroes only of the finite order.

Indeed, then (2.25) will be replaced by $\mathsf{mes}_1(\Lambda(\theta) \cap \Sigma_\lambda) \leq C\gamma^\nu$, $\nu = 1/(q+1)$ with q the maximal order of zeroes of $\varkappa(s)$.

General Case: Gauge Transformation. Consider now the general case $d \geq 2$. In this case due Conditions 1.2, 1.5 and 1.6 we can cover $\Lambda \cap \Omega_\tau$ by Λ^*,

$$\Lambda \cap \Omega_\tau \subset \Lambda^* = \bigcup_{1 \leq j \leq d-1} \Lambda_j^*, \tag{2.29}$$

defined as:

(2.30) Let $\xi \in \Omega_\tau$; then $\xi \in \Lambda_j^*$ iff there exist $\theta_1, \dots, \theta_j \in \Theta'_K$ which are linearly independent and such that $\xi \in \Lambda_{\delta_j}(\theta_k)$ for all $k = 1, \dots, j$,

where $0 < \delta = \delta_1 < \delta_2 < \dots < \delta_{d-1}$ are arbitrarily fixed and we chose sufficiently small $\sigma > 0$ afterwards.

Further, due to Conditions 1.2, 1.5, 1.6 and (1.16) $\Lambda_{d-1}^* \cap \Omega_\tau$ could be covered by no more than γ_{d-1}-vicinities of some points ξ_ι, $\iota = 1, \dots, \omega^g$, $g = g(d)$. Recall that $\Omega_\tau := \{\xi \colon |A^0(\xi) - \tau| \leq C_0\varepsilon + h^{1-\varsigma}\}$.

Consider some connected component Ξ of Λ_j^*. Let some point $\bar{\xi}$ of it belong to $\bigcap_{1 \leq k \leq j} \Lambda_{\delta_j}(\theta_k) \cap \Omega_\tau$ with linearly independent $\theta_1, \dots, \theta_j$. Observe that $\mathsf{diam}(\bigcap_{1 \leq k \leq j} \Lambda_{\delta_j}(\theta_k) \cap \Omega) \leq c\gamma_j$ due to strong convexity assumption (1.16). Then this set either intersects or does not intersect with $\Lambda_{j+1}^* \cap \Omega$. In the former case we include it to Λ_{j+1}^* and exclude it from Λ_j^*.

After we redefined Λ_j^* we arrive to the following proposition:

Proposition 2.11. *Equation* (2.29) *still holds where now each connected component* Ξ *of* Λ_j^* *has the following properties:*

(i) $\operatorname{diam}\Xi \le c\gamma_j$.

(ii) There exist linearly independent $\theta_1, \dots, \theta_j \in \Theta'_K$, *such that for each* $\xi \in \Xi$ $|\langle \nabla_\xi A^0(\xi), \theta\rangle| \le c_j\gamma_j$ *for all* $\theta \in \mathfrak{V} \cap (\Theta'_K \setminus 0)$ *and* $|\langle \nabla_\xi A^0(\xi), \theta\rangle| \ge \epsilon_j\gamma_{j+1}$ *for all* $\theta \in \Theta'_K \setminus \mathfrak{V})$ *with* $\mathfrak{V} = \operatorname{Span}(\theta_1, \dots, \theta_j)$.

Now we generalize Proposition 2.7:

Proposition 2.12. *Let* $Q = Q(hD)$ *with the symbol supported in the connected component* Ξ *of* Λ_j^*, *corresponding to subspace* $\mathfrak{V}$, *and satisfying* (2.3). *Then there exists a pseudo-differential operator* $P = P(x, hD)$ *with the symbol, satisfying* (2.18) *and such that*

$$\big(e^{-i\varepsilon h^{-1}P} A e^{i\varepsilon h^{-1}P} - A''\big) Q \equiv 0 \tag{2.31}$$

modulo operator from $\mathscr{H}^m$ *to* $\mathscr{L}^2$ *with the operator norm* $O(h^{3M})$, *where* $A'' = A^0 + \varepsilon B''(x, hD)$, *where* B'' *is an operator with Weyl symbol*

$$B''(x,\xi) = \sum_{\theta \in \Theta'_K \cap \mathfrak{V}} b_{\mathfrak{V},\theta}(\xi) e^{i\langle\theta,x\rangle}. \tag{2.32}$$

Proof. The proof obviously generalizes the proof of Proposition 2.7. We eliminate all $\theta \notin \mathfrak{V}$ exactly in the same way as it was done there. □

General Case: Propagation.

Proposition 2.13. *Let* $Q_j = Q_j(hD)$ *with the symbols, satisfying* (2.3) *and let symbol of* Q_1 *be supported in* Λ_j^* .

Let $\operatorname{dist}(\operatorname{supp}(Q_1), \operatorname{supp}(Q_2)) \ge C_0\gamma_j$. *Then* $\|Q_2 e^{ih^{-1}tA} Q_1\| = O(h^{2M})$ *for* $|t| \le T_* = h^{-M}$.

Proof. In virtue of Proposition 2.9 it is sufficient to consider $\operatorname{supp}(Q_1)$ belonging to the connected component Ξ' of Λ_j^*. Indeed, the values of $\delta_1, \dots, \delta_{d-1}$ are arbitrarily small.

One can prove easily that the operator norm of $Q_2 e^{\pm i\varepsilon h^{-1}P} Q_1$ are $O(h^{2M})$. We need to prove that the operator norm of $Q_2 e^{\pm ih^{-1}tA''} Q_1$ is also $O(h^{2M})$. In the coordinates $(x'; x'') \in \mathfrak{V} \oplus (\mathbb{R}^d \ominus \mathfrak{V})$ we observe that the propagation speed is only along $\mathfrak{V}$ as long as it remains in $\epsilon\gamma_j$ vicinity of $\mathsf{supp}(Q_1)$. The proof is similar to the proof of Proposition 2.2 and we leave it to the reader.

However propagation is confined to $\Omega'_\tau := \{\xi\colon |A^0(\xi)-\tau| \le C\varepsilon + 2h^{1-\varsigma}\})$ and due to (1.16) it remains in that vicinity as $\varsigma < \delta$. □

Now we arrive to the following proposition:

Proposition 2.14. *Let* Q_1, Q_2 *satisfy* (2.3) *and* $\mathsf{supp}(Q_1) \subset \Omega$. *Then for* $T_* \le T \le T^*$

$$F_{t\to h^{-1}\tau}\bigl(\chi_T(t) Q_{2x} u(x,y,t)\, {}^tQ_{1y}\bigr) = O(h^{2M}). \tag{2.33}$$

Proof. It is standard, due to Proposition 2.13, microhyperbolicity condition and the results of Chapter 2 of [Ivr1] we conclude that if $|\ell| = 1$ and

$$\langle \ell, \nabla_\xi A^0(\xi)\rangle \ge \epsilon_0 \qquad \forall \xi \in \mathsf{supp}(Q_1) \tag{2.34}$$

and

$$\langle \ell, x-y\rangle \le \epsilon_1 T \qquad \forall x \in \mathsf{supp}(\phi_1),\ \ y \in \mathsf{supp}(\phi_2), \tag{2.35}$$

then $\|\phi_2 e^{ih^{-1}tA} Q_1 \phi_2\| = O(h^{2M})$ for $T \le t \le 2T$.

This implies (2.33) provided $\mathsf{diam}(\mathsf{supp}(Q_1)) \le \epsilon$. But then for (2.33) we can drop this assumption. □

2.6 End of the Proof

Now we conclude that

$$F_{t\to h^{-1}\tau}\bigl([\bar\chi_T(t) - \bar\chi_{T_*}(t)] Q_{2x} u(x,y,t)\, {}^tQ_{1y}\bigr)\bigr|_{x=y} = O(h^{2M}) \tag{2.36}$$

and since

$$F_{t\to h^{-1}\tau}\bigl(\bar\chi_T(t) Q_{2x} u(x,y,t)\, {}^tQ_{1y}\bigr)\bigr|_{x=y} = \sum_{0\le n\le M} \kappa'_n(x,\varepsilon) h^{1-d+n} + O(h^{M+1}) \tag{2.37}$$

holds for $T = T_*$, it also holds for $T = T^*$.

Finally, Hörmander's Tauberian theorem implies Theorem 1.8.

3 Generalizations and Discussion

3.1 Matrix Operators

Consider now $n \times n$-matrix operators A^0 and B; then (1.2) should be understood in the matrix sense. Assume that

(3.1) Symbol $A^0(\xi)$ has only simple eigenvalues $a_1^0(\xi), \dots, a_n^0(\xi)$, which also satisfy (1.4) and (1.16).

Then there exists a unitary transformation $R^0 = R(\xi)$, such that $R^{0\,\dagger}(\xi)A^0(\xi)R^0(\xi) = \mathsf{diag}(a_1^0(\xi), \dots, a_n^0(\xi))$.

Then one can prove easily, that there exists a unitary operator $R(x, hD) = R^0(hD) + \varepsilon R'(x, D)$, such that $R^*AR = \mathsf{diag}(a_1, \dots, a_n)$, where $a_j = a_j(x, hD) = a_j^0(hD) + \varepsilon b_j(x, hD)$ (and we assume as before that (2.17) holds.

If Conditions 1.2–1.6 are fulfilled for $A(x, hD)$, then they are also fulfilled for $a_j(x, hD)$ and we can apply the same propagation arguments as before and Theorem 1.8 extends to such operators provided conditions (1.4) and (1.16) are fulfilled for $a_j(x, hD)$ with $j = 1, \dots, n$.

Let us replace (1.2) by more general ellipticity assumption

$$|A^0(\xi)v| \geq \epsilon |\xi|^m |v| \qquad \forall v \in \mathbb{C}^n\ \forall \xi\colon |\xi| \geq C_0. \tag{3.2}$$

Then we cannot restrict $e(x, y, \lambda)$ to $x = y$ but we can restrict $e(x, y, \lambda, \lambda')$, the Schwartz kernel of the difference of the corresponding projectors.

Theorem 1.8 trivially extends to such operators, if instead of $e(x, x, \lambda)$ we consider $e(x, x, \lambda, \lambda')$ provided conditions (1.4) and (1.16) are fulfilled for $a_j(x, hD)$ with $j = 1, \dots, n$ and for both λ and λ'. It also extends to

$$\int e(x, y, \lambda, \lambda')\phi(\lambda')\, d\lambda', \qquad \phi \in \mathscr{C}_0^\infty(\mathbb{R}), \tag{3.3}$$

provided conditions (1.4) and (1.16) are fulfilled for $a_j(x, hD)$ with $j = 1, \dots, n$ for λ.

Remark 3.1. Our reduction construction fails in the case of a scalar operator A^0 and a matrix operator B unless either $\varepsilon = h^{1+\delta}$ or the principal symbol of B satisfies some very restrictive condition. Therefore for a matrix operator A^0 with the eigenvalues of $A^0(\xi)$ of constant multiplicities our construction works only under similar assumptions.

3.2 Perturbations

Consider operators in question, perturbed by $\varepsilon V(x, hD)$ where $V(x, \xi)$ decays as $|x| \to \infty$. Such perturbations do not affect $\mathsf{N}_h(\lambda)$, but they do affect $e_h(x, x, \lambda)$.

Decaying Perturbations. We start from the easy case

$$A = A^0(hD) + \varepsilon V(x, hD), \tag{3.4}$$

where

$$|D_\xi^\alpha D_x^\beta V(x, \xi)| \le c_{\alpha\beta}(|\xi| + 1)^m (|x| + 1)^{-\delta - |\beta|} \qquad \forall \alpha, \beta\ \forall x, \xi. \tag{3.5}$$

First of all, we claim that

(3.6) Under assumption (3.7) below the propagation speed with respect to ξ does not exceed $c\varepsilon(|x| + 1)^{-\delta}$.

Indeed, note first that due to Proposition 2.2 the propagation speed with respect to ξ does not exceed $c\varepsilon$. Next, consider domain $\{x\colon |x| \asymp r\}$ with $r \ge 1$. Scaling $x \mapsto x/r$, $t \mapsto t/r$ we get a domain $\{x\colon |x| \asymp 1\}$, $h \mapsto \hbar = h/r$ and we need to prove that after this scaling the propagation speed with respect to ξ does not exceed $\nu = c\varepsilon r^{-\delta}$, on the time interval $\{t\colon |t| \le 1\}$.

To prove this we can apply Proposition 2.2 but ewe need to have the microlocal uncertainty principle fulfilled: $\nu \ge \hbar^{1-\sigma}$ with $\sigma > 0$, where ν is a shift with respect to ξ. This inequality is equivalent to $\varepsilon r^{-\delta} \ge h^{1-\sigma} r^{-1+\sigma}$ i.e. $\varepsilon r^{1-\sigma-\delta} \ge h^{1-\sigma}$ and it suffice to have

$$\delta < 1, \qquad \varepsilon \ge h^{1-\sigma} \quad \text{with} \quad \sigma > 0. \tag{3.7}$$

To join different time intervals one can use the technique of Subsection 12.7.6.

Consider now ξ in the vicinity of $\bar{\xi}$ and x with $|x| \le c$. Then as long as $|\xi - \bar{\xi}| \le \epsilon$ with small enough constant $\epsilon > 0$, evolution goes away from 0 with the speed $\asymp 1$, so we are in the zone $\{x\colon |x| \asymp |t|\}$ and in this zone the propagation speed with respect to ξ does not exceed $c\varepsilon r^{-1-\delta}$, and therefore $|\xi - \bar{\xi}| \le c\varepsilon \int_1^\infty t^{-1-\delta}\, dt \le c\varepsilon$ and this is less that $\epsilon/2$ as $\varepsilon \le \epsilon_0$.

We can also consider evolution which starts from x with $|x| \ge 1$. Then the same arguments work albeit with $r \asymp |t - t^*|$ for some t^* with $|t^*| \le c|x|$.

Then we arrive to

Theorem 3.2. *Consider operator* (3.4) *with* V *satisfying* (3.5). *Let microhyperbolicity condition* (1.4) *on the energy level* λ *be fulfilled and* $\varepsilon \le \epsilon_0$. *Then the complete spectral asymptotics* (1.29) *holds.*

Hybrid Perturbations. Now we consider the hybrid operators, containing both εB and εV. However, trying to eliminate εB by the same approach as in Subsubsection 2.5.2, we get an another type of terms, and it is only natural to consider them being in the operator from the beginning:

$$A = A^0(hD) + \varepsilon\bigl(B(x, hD) + V(x, hD)\bigr), \tag{3.8}$$

where

$$V(x,\xi) = \sum_{\theta\in\Theta} e^{i\langle\theta,x\rangle} V_\theta(x,\xi), \tag{3.9}$$

$$|D_\xi^\alpha D_x^\beta V(x,\xi)| \le c_{\alpha\beta}(|\xi|+1)^m(|x|+1)^{-\delta} \quad \forall \alpha,\beta\ \forall x,\xi. \tag{3.10}$$

We impose condition

Condition 3.3. *For each* ω *and* L *for the same set* Θ' *as before there exists*

$$V'(x,\xi) = \sum_{\theta\in\Theta'} e^{i\langle\theta,x\rangle} V'_\theta(x,\xi), \tag{3.11}$$

such that

$$\|D_x^\alpha D_\xi^\beta \bigl(V - V'\bigr)\|_{\mathscr{L}^\infty} \le \omega^{-L}(|\xi|+1)^m \tag{3.12}$$

and

$$|D_x^\alpha D_\xi^\beta V'_\theta| \le c_{Ls\alpha\beta}(|x|+1)^{-1-\delta-|\alpha|}(|\theta|+1)^{-s} \tag{3.13}$$

$$\forall \alpha,\beta\colon |\alpha|\le L, |\beta| \le L\ \forall s.$$

Non-Resonant Zone. We deal with the purely exponential terms in our standard way and with the hybrid terms as if they were purely exponential (i.e. as if V'_θ were not depending on x), then a new kind of terms will be produced: they acquire factor $h(A^0(\xi+\theta h/2) - A^0(\xi-\theta h/2))^{-1}$ and the derivative with respect to x to V'_θ.

Eventually we end up with the operator of the same type (3.8) with $B(x,\xi)$ replaced by $B''(\xi)$ and with $V_\theta(x,\xi)$ replaced by $V''_\theta(x,\xi)$, such that

$$|D_\xi^\alpha D_x^\beta V''_\theta(x,\xi)| \le C_{n\alpha\beta}\varepsilon^{k+1}\gamma^{-2k-n-|\alpha|}(|x|+1)^{-n-\delta-|\beta|}$$

with $n+k\ge 3K$.

Then

$$|D_\xi^\alpha D_x^\beta\bigl[V''_\theta(x,\xi)e^{i\langle\theta,x\rangle}\bigr]|\le C_{s\alpha\beta}\varepsilon^{k+1}\gamma^{-2k-n-|\alpha|}(|x|+1)^{-n-\delta}(|\theta|+1)^{|\beta|};$$

recall that $|\theta|\le CKh^{-\sigma}$.

Let us pick up $\gamma=h^\delta$ with $\delta=\vartheta/6K$. Then, ignoring therms with $k\ge K$ which are negligible, and following the proof of (3.6), we can recover the same statement for the operator after transform, and, finally, to the analogue of Proposition 2.9.

Resonant Zone. If $d=2$ we arrive to the analogue of Proposition 2.2 in the virtue of the we arguments as in Subsubsection 2.5.1.

If $d\ge 3$ we apply the reduction, similar to one, used in Subsubsection 2.5.3, and arrive again to operator of the type (3.8) with B replaced by $B''(x,\xi')$ and with $V_\theta(x,\xi)$ replaced by $V''_\theta(x,\xi)$.

Then we observe that the shift in direction $\mathbb{R}^d\ominus\mathfrak{V}$ does not exceed $c\varepsilon^{\delta/2}$ and if it is $\ll\gamma^2$ we arrive to the analogue of Proposition 2.13. It is doable by the choice of really small $\sigma_1<...<\sigma_{d-1}$. Then we arrive to the analogue of Proposition 2.14 and, finally, to

Theorem 3.4. *Let A be a self-adjoint operator* (3.8)*, where A^0 satisfies* (1.1)*,* (1.2)*,* (1.4) *and* (1.16) *and B satisfies* (1.1)*, V satisfies* (3.9) *and* (3.10)*.*

Let Conditions 1.2–3.3 be fulfilled. Then for $|\tau-\lambda|<\epsilon$, $\varepsilon\le h^\vartheta$, $\vartheta>0$ asymptotics (1.29) *holds.*

3.3 Differentiability

It also follows from Corollary 1.9 that

$$\frac{1}{\nu}\Bigl[\mathsf{N}_{h,\varepsilon}(\tau+\nu)-\mathsf{N}_{h,\varepsilon}(\tau)\Bigr]=\frac{1}{\nu}\Bigl[\mathcal{N}_{h,\varepsilon}(\tau+\nu)-\mathcal{N}_{h,\varepsilon}(\tau)\Bigr]+O(h^\infty)\tag{3.14}$$

provided $\nu\ge h^M$, where $\mathcal{N}_{h,\varepsilon}(\tau)$ is the right-hand expression of (1.30).

The question remains, if (3.14) holds for smaller ν, in particular, if it holds in $\nu\to 0$ limit? If the latter holds, then

$$\frac{\partial}{\partial\tau}\mathsf{N}_{h,\varepsilon}(\tau)=\frac{\partial}{\partial\tau}\mathcal{N}_{h,\varepsilon}(\tau)+O(h^\infty)\tag{3.15}$$

and we call the left-hand expression the *density of states*.

It definitely is not necessarily true, at least in dimension 1. From now on we consider only asymptotics with respect to $\tau \to +\infty$. Let $A = \Delta + V(x)$ with periodic V. It is well-known that for $d = 1$ and generic periodic V all spectral gaps are open which contradicts to

$$\frac{\partial}{\partial\tau}\mathsf{N}(\tau) = \frac{\partial}{\partial\tau}\mathcal{N}(\tau) + O(\tau^{-\infty}). \tag{3.16}$$

On the other hand, this objection does not work in case $d \geq 2$ since only several the lowest spectral gaps are open (Bethe-Sommerfeld conjecture, proven in [PS]).

Assume for simplicity, that $A = \Delta + V$ has no negative eigenvalues; then we can apply wave operator method[8]. We consider $u(x, y, t)$, the Schwartz kernel of $\cos(\sqrt{A}t)$,

$$u(x, y, t) = \int \cos(t\tau)\, d_\tau e(x, y, \tau^2). \tag{3.17}$$

Then, for compactly supported V [9]

$$u(x, y, t) = \begin{cases} O(e^{-\epsilon|t|}) & \text{for odd } \ d, \\ O(|t|^{-d}) & \text{for even } \ d \end{cases} \tag{3.18}$$

as $|x| + |y| \leq c$, $|t| \to +\infty$ and $\frac{\partial}{\partial\tau} e(x, x, \tau^2)$ could be completely restored by inverse cos-Fourier transform, without any Tauberian theorem, and we arrive to asymptotics of $\frac{\partial}{\partial\tau} e(x, x, \tau^2)$. Moreover, we can differentiate complete asymptotics of the *Birman-Krein spectral shift function*

$$\xi(\tau) := \int \bigl(e(x, x, \tau^2) - e^0(x, x, \tau^2)\bigr)\, dx \sim \sum_{n\geq 0} \bar{\kappa}_n \tau^{-d+n}, \tag{3.19}$$

with

$$\bar{\kappa}_n := \int (\kappa_n(x) - \kappa_n^0)\, dx, \tag{3.20}$$

where $e^0(x, y, \tau)$ and κ_n^0 correspond to $A^0 = \Delta$. In the case of $A = \Delta$ in the exterior of smooth, compact and non-trapping obstacle and $A^0 = \Delta$ in $\mathbb{R}^d$ such asymptotics was derived in [PP].

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[8] It could be applied without this assumption, but with tweaking.

[9] It, probably could be proven for V, decaying fast enough at infinity

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Complete Differentiable Semiclassical Spectral Asymptotics*,†

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Abstract

For an operator $A := A_h = A^0(hD) + V(x, hD)$ with a "potential" V decaying as $|x| \to \infty$ we establish under certain assumptions the complete and differentiable with respect to τ asymptotics of $e_h(x, x, \tau)$ where $e_h(x, y, \tau)$ is the Schwartz kernel of the spectral projector.

1 Introduction

Consider a self-adjoint matrix operator

$$A := A_h = A^0(hD) + V(x, hD), \tag{1.1}$$

where

$$|D_\xi^\beta A^0(\xi)| \le c_{\alpha\beta}(|\xi| + 1)^m \qquad \forall\beta\ \forall\xi \tag{1.2}$$

and

$$A^0(\xi) \ge c_0|\xi|^m - C_0 \qquad \forall\xi. \tag{1.3}$$

We assume that $A^0(\xi)$ is *ξ-microhyperbolic at energy level λ*, i.e. for each ξ there exists a direction $\ell(\xi)$ such that $|\ell(\xi)| \le 1$ and

$$(\langle \ell(\xi), \nabla_\xi\rangle A^0(\xi)v, v) + |(A^0(\xi) - \lambda)v| \ge \epsilon_0|v|^2 \qquad \forall v. \tag{1.4}$$

Further, we assume that $V(x, \xi)$ is a real-valued function, satisfying

$$|D_\xi^\alpha D_x^\beta V(x, \xi)| \le c_{\alpha\beta}(|\xi| + 1)^m(|x| + 1)^{-\delta-|\beta|} \qquad \forall\alpha, \beta\ \forall x, \xi \tag{1.5}$$

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and

$$|D_\xi^\alpha D_x^\beta V(x,\xi)| \le \varepsilon \qquad \forall \alpha,\beta\colon |\alpha|+|\beta|\le 1\ \forall x,\xi. \tag{1.6}$$

Our main theorem is

Theorem 1.1. *Let conditions* (1.2)– (1.4) *and* (1.6) *with sufficiently small constant* $\varepsilon>0$ *be fulfilled. Then*

(i) The complete spectral asymptotics holds for $\tau\colon |\tau-\lambda|\le\epsilon$*:*

$$e_h(x,x,\tau)\sim\sum_{n\ge 0}\kappa_n(x,\tau)h^{-d+n} \tag{1.7}$$

where $e_h(x,y,\tau)$ *is the Schwartz kernel of the spectral projector* $\theta(\tau-A_h)$ *of* A_h*.*

(ii) This asymptotics is <u>*infinitely differentiable*</u> *with respect to* τ*.*

Remark 1.2. (i) Statement (i) was sketched under much more restrictive assumptions in Theorem 3.2 of [Ivr3]; however we provide here more detailed exposition.

(ii) In Theorem 2.8 we provide the dependence of the remainder on $|x|$.

(iii) This asymptotics is also infinitely differentiable with respect to x but it is really easy.

Differentiability and completeness of the spectral asymptotics are really different. F.e. for operators with almost periodic with respect to x perturbation $V(x,hD)$ the spectral asymptotics are complete (see [Ivr3] and references there) but in dimension 1 it is not necessarily differentiable even once due to spectral gaps. Furthermore, if we perturb an operator we study in this paper by an appropriate "negligible" operator (i. e. with $O(h^\infty)$ norm), the absolutely continuous spectrum on the segment $[\lambda_-,\lambda_+]$ with $\lambda_\mp=\lambda+O(h^\infty)$ will be replaced by an eigenvalue of the infinite multiplicity and then the spectral asymptotics will complete albeit non-differentiable even once.

To establish spectral asymptotics we apply the "hyperbolic operator method"; namely, let us consider the Schwartz kernel of the propagator $e^{ih^{-1}tA_h}$:

$$u:=u_h(x,y,t)=\int e^{ih^{-1}t\tau}\,d_\tau e_h(x,y,\tau). \tag{1.8}$$

Then under ellipticity and microhyperbolicity conditions (1.3) and (1.4)

$$F_{t\to h^{-1}\tau}\bar{\chi}_T(t)u_h(x,x,t) \sim \sum_{n\geq 0}\kappa'_n(x,\tau)h^{1-d+n}, \tag{1.9}$$

where here and below $\chi\in\mathscr{C}_0^\infty([-1,-\frac{1}{2}]\cup[\frac{1}{2},1])$, $\bar{\chi}\in\mathscr{C}_0^\infty([-1,1])$, $\bar{\chi}(t)=1$ on $[-\frac{1}{2},\frac{1}{2}]$, $\chi_T(t)=\chi(t/T)$ etc, $\kappa'_n(x,\tau)=\partial_\tau\kappa_n(x,\tau)$, and $T=T_*>0$ is a small constant here.

Then, due to Tauberian theorem we arrive to the spectral asymptotics with the remainder estimate $O(h^{1-d})$. Next, under different assumptions one, using propagation of singularities technique, can prove that

$$|F_{t\to h^{-1}\tau}\chi_T(t)u_h(x,x,t)| = O(h^\infty) \tag{1.10}$$

for all $T\in[T_*,T^*]$. Then (1.9) holds with $T=T^*$ and again, due to Tauberian theorem, we arrive to the spectral asymptotics with the remainder estimate $O(T^{*\,-1}h^{1-d})$ (provided $T^*=O(h^{-K})$). In particular, if (1.10) holds provided $T^*=h^{-\infty}$, we arrive to complete spectral asymptotics. This happens f.e. in the framework of [Ivr3].

However we do not have Tauberian theorems for the derivatives (with respect to τ) and we need to use an inverse Fourier transform and its derivatives

$$\partial_\tau^n e_h(x,x,\tau) = (2\pi h)^{-1}\int_{\mathbb{R}} e^{-ih^{-1}\tau t}(-ih^{-1}t)^{n-1}u_h(x,x,t)\,dt \tag{1.11}$$

for $n\geq 1$. If we insert a factor $\bar{\chi}_T(t)$ into integral, we will get exactly n-th derivative of the right-hand expression of (1.7). However we need to estimate the remainder

$$(2\pi h)^{-1}\int_{\mathbb{R}} e^{-ih^{-1}\tau t}(-ih^{-1}t)^{n-1}(1-\bar{\chi}_T(t))u_h(x,x,t)\,dt \tag{1.12}$$

and to do this we need to properly estimate the left-hand expression of (1.10) for all $T\geq T_*$ (rather than for $T\in[T_*,T^*]$).

To achieve this we will use a more subtle propagation technique and prove that for $T\geq T_*(R)$ the left-hand expression of (1.10) is $O((h/T)^\infty)$, provided $|x|\leq R$.

2 Proofs

2.1 Preliminary Remarks

Observe that, due to assumptions (1.6) and (1.5) a propagation speed with respect to ξ does not exceed $\min\bigl(\varepsilon,\ C(|x|+1)^{-1-\delta}\bigr)$ and one can prove easily, that for for a generalized Hamiltonian trajectory[1)] $(x(t),\xi(t))$ on energy level $\tau\le c$

$$\Sigma_\tau \coloneqq \{(x,\xi)\colon\ \operatorname{Ker}(A(x,\xi)-\tau)\ne\{0\}\} \tag{2.1}$$

with $A(x,\xi)=A^0(\xi)+V(x,\xi)$ we have $|\xi(t)-\xi(0)|\le\varepsilon'$ for all t with $\varepsilon'=\varepsilon'(\varepsilon)\to 0$ as $\varepsilon\to 0$ and therefore

(2.2) Let conditions (1.2)–(1.4), (1.5) and (1.6) with $\varepsilon=\varepsilon(\varepsilon')>0$ with arbitrarily small ε' be fulfilled. Then for a generalized Hamiltonian trajectory $(x(t),\xi(t))$ on Σ_τ

$$|\xi(t)-\xi(0)|\le\varepsilon'\quad\text{and}\quad |x(t)-x(0)|\ge\epsilon_2|t|\qquad\forall t\in\mathbb{R}. \tag{2.3}$$

Then we conclude immediately that inequality

$$|F_{t\to h^{-1}\tau}\chi_T(t)u_h(x,x,t)|\le C'_s(T)h^s \tag{2.4}$$

holds for arbitrarily constant $T>0$.

Combining with (1.9) for small constant T we conclude that

(2.5) Let conditions (1.2)–(1.4), (1.5) and (1.6) with sufficiently small constant $\varepsilon>0$ be fulfilled. Then asymptotic decomposition (1.9) holds with an arbitrarily large constant T.

2.2 Propagation and Local Energy Decay

First we have the finite speed with respect to x propagation:

Proposition 2.1. *For $\tau\le c$ the following estimate holds*

$$|F_{t\to h^{-1}\tau}\Bigl(\chi_T(t)u(x,y,t)\Bigr)|\le C'_s h^s R^{-s}\qquad \forall x,y\colon |x-y|\ge C_0T,\ |x|+|y|\asymp R. \tag{2.6}$$

1) For a definition of the generalized Hamiltonian trajectory see Definition 2.2.8 of [Ivr1].

Proof. In the zone $\{x\colon |x|\asymp R\}$ we can apply scaling $x\mapsto xR^{-1}$, $t\mapsto tR^{-1}$, $h\mapsto hR^{-1}$ and apply the standard theory of Chapter 2 of [Ivr1]. The rest is trivial. □

Next, we consider $R\le \epsilon_1 T$ and apply energy estimate method to prove the local energy decay. Observe that one can select smooth $\ell(\xi)$ in condition (1.4). Consider operator $L^0(x,hF)$ with Weyl symbol $-\langle x,\ell(\xi)\rangle$ and $L(x,hD;t)=L^0+\varepsilon t$.

Then

$$2h^{-1}\operatorname{Re} i((hD_t-A)v,Lv)_{\Omega_T} = (Lv,v)\bigr|_{t=0}^{t=T} - \operatorname{Re} ih^{-1}([hD_t-A,L]v,v)_{\Omega_T} = (Lv,v)\bigr|_{t=0}^{t=T} -\varepsilon\|v\|^2_{\Omega_T} + \operatorname{Re}(ih^{-1}[A,L]v,v)_{\Omega_T}, \tag{2.7}$$

where $\|.\|_\Omega$ and $(.,.)_\Omega$ are a norm and an inner product in $\mathscr{L}^2(\Omega)$ with $\Omega=\Omega_T=\mathbb{R}^d\times[0,T]\ni(x,t)$. Indeed, writing the left-hand expression as

$$ih^{-1}\bigl[((hD_t-A)v,Lv)_{\Omega_T}-(L,(hD_t-A)v)_{\Omega_T}\bigr]=\\ ih^{-1}\bigl[(L(hD_t-A)v,v)_{\Omega_T}-((hD_t-A)L,v)_{\Omega_T}\bigr]+(Lv,v)\bigr|_{t=0}^{t=T}$$

because $L^*=L$, we arrive to (2.7).

In virtue of (1.5) and (1.6) for sufficiently small constant ε and for $h\le h_0(\varepsilon_1)$ the operator norm of $h^{-1}[V,L]$ from $\mathscr{H}^m(\mathbb{R}^d)$ to $\mathscr{L}^2(\mathbb{R}^d)$ does not exceed ε_1 with $\varepsilon_1=\varepsilon_1(\varepsilon)\to 0$ as $\varepsilon\to 0$, and then due to the microhyperbolicity assumption we conclude that

$$\operatorname{Re}(ih^{-1}[A,L]v,v)\ge(\epsilon_0-2\varepsilon_1)\|v\|^2 - C\|(A-\tau)v\|^2 \tag{2.8}$$

for both $\mathbb{R}^d$ and Ω_T.

Let us plug into (2.7) $v=\varphi_\varepsilon(A-\tau)e^{ihtA}w$ where $\varphi\in\mathscr{C}_0^\infty([-1,1])$, $0\le\varphi\le 1$; then for sufficiently small constant $\varepsilon>0$ we arrive to

$$\epsilon\|v\|^2_{\Omega_T}+(Lv,v)\bigr|_{t=T}\le (Lv,v)\bigr|_{t=0}. \tag{2.9}$$

On the other hand,

$$\operatorname{Re}(Lv,v)|_{t=T}\ge \varepsilon T\|v\|^2 - C\||x|^{\frac12}v\|^2 \tag{2.10}$$

with

$$\||x|^{\frac{1}{2}}v\|^2 = \||x|^{\frac{1}{2}}v\|^2_{B(0,R)} + \||x|^{\frac{1}{2}}v\|^2_{B(0,R')\setminus B(0,R)} + \||x|^{\frac{1}{2}}v\|^2_{\mathbb{R}^d\setminus B(0,R')}$$

with $R' = C_0T$ and therefore for $R \le \varepsilon T$

$$\operatorname{Re}(Lv, v)|_{t=T} \ge \varepsilon T\|v\|^2 - CR'\|v\|^2_{B(0,R')\setminus B(0,R)} - \||x|^{\frac{1}{2}}v\|^2_{\mathbb{R}^d\setminus B(0,R')}. \tag{2.11}$$

Observe that

$$|(Lv, v)|_{t=0} \le C\Big(\|v_0\|^2 + \||x|^{\frac{1}{2}}v_0\|^2\Big)$$

and then (2.9) and (2.10) imply that if $R \le \varepsilon T$ then

$$\|v\|^2_{B(0,r)} \le \sigma\|v_0\|^2 + CT^{-1}\Big(\||x|^{\frac{1}{2}}v\|^2_{\mathbb{R}^d\setminus B(0,R')} + \|v_0\|^2 + \||x|^{\frac{1}{2}}v_0\|^2\Big) \tag{2.12}$$

with $\sigma < 1$ and $v|_0 = v|_{t=0}$; recall that $\|v\| = \|v_0\|$.

Recall that $v = e^{ih^{-1}tA}\varphi_\varepsilon(A-\tau)\psi_R(x)w$ where we plugged $\psi_R w$ instead of w, $\psi \in \mathscr{C}_0^\infty(B(0,1))$, $0 \le \psi \le 1$ and $\psi = 1$ in $B(0,\frac{1}{2})$.

One can prove easily that $Q = \varphi_\varepsilon(A-\tau)$ is an operator with Weyl symbol $Q(x,\xi)$, satisfying

$$|D_\xi^\alpha D_x^\beta Q| \le C_{\alpha\beta}\varepsilon^{-|\alpha|-|\beta|}(|x|+1)^{-|\beta|}.$$

Then $\|v_0\|_{\mathbb{R}^d\setminus B(0,2R)} \le C(h/R)^s\|w\|$ and therefore $\||x|^{\frac{1}{2}}v_0\|^2 \le 2R\|w\|^2$. Further, then Proposition 2.1 implies that $\||x|^{\frac{1}{2}}v\|^2_{\mathbb{R}^d\setminus B(0,R')} \le C(h/T)^s\|w\|$ provided or $R' \ge C_0T$ with sufficiently large C_0 and we arrive to

Proposition 2.2. *In the framework of Theorem 1.1*

$$\|\psi_R e^{ih^{-1}TA}\varphi_\varepsilon(A-\lambda)\psi_R\| < 1 \tag{2.13}$$

provided $\varepsilon T \ge R \ge 1$.

While this statement looks weak, it will lead to much stronger one:

Proposition 2.3. *In the framework of Theorem 1.1*

$$\|\psi_R e^{ih^{-1}TA}\varphi_\varepsilon(A-\lambda)\psi_R\| \le C_sR^sT^{-s} \tag{2.14}$$

provided $T \ge C_0R$, $R \ge 1$.

Proof. We want to prove by induction that

$$\|\psi_R e^{inh^{-1}TA}\varphi_\varepsilon(A-\lambda)\psi_R\| \le C\nu^N + C_s nR^s T^{-s} \tag{2.15}$$

with $\nu<1$.

Assuming that for n we have (2.15), we apply the previous arguments on the interval $[nt,(n+1)T]$ to $v=e^{ih^{-1}tA}\varphi_\varepsilon(A-\lambda)\psi_{R/2}e^{ih^{-1}nTA}\psi_R w$ and derive an estimate

$$\|\psi_R e^{ih^{-1}tA}\varphi_\varepsilon(A-\lambda)\psi_{R/2}e^{ih^{-1}nTA}\psi_R w\| \le \\ \nu\|\varphi_\varepsilon(A-\lambda)\psi_R e^{ih^{-1}nTA}\psi_R w\| + C'_K(h/R)^K\|w\| \tag{2.16}$$

with $\nu<1$.

To make a step of induction we weed to estimate the norm of

$$\psi_R e^{ih^{-1}tA}\varphi_\varepsilon(A-\lambda)(1-\psi_{R/2})e^{ih^{-1}nTA}\psi_R w = \\ \psi_R e^{ih^{-1}tA}\varphi_\varepsilon(A-\lambda)(1-\psi_{R/2})Q^+e^{ih^{-1}nTA}\psi_R + \\ \psi_R e^{ih^{-1}tA}\varphi_\varepsilon(A-\lambda)(1-\psi_{R/2})Q^-e^{ih^{-1}nTA}\psi_R, \tag{2.17}$$

with $Q^\pm=Q^\pm(x,hD)$, $Q^++Q^-=I$ to be selected to ensure that

(2.18) Generalized Hamiltonian trajectories on Σ_τ, starting as $t=0$ from $\operatorname{supp}(Q^\pm)\cap\operatorname{supp}(1-\psi_{R/2})$ in the positive (negative) time direction, remain in the zone $\{|x|\ge\epsilon_1R+\epsilon_2|t|\}$.

Then we show that

$$\|\psi_R e^{ih^{-1}tA}\varphi_\varepsilon(A-\lambda)(1-\psi_{R/2})Q^+\| \le C_s(h/R)^s \tag{2.19}$$

and

$$\|\varphi_\varepsilon(A-\lambda)(1-\psi_{R/2})Q^-e^{ih^{-1}nTA}\psi_R\| \le C_s(h/R)^s. \tag{2.20}$$

To achieve that consider $A^0(\xi)$ and for each ξ in the narrow vicinity $\mathcal{W}$ of Σ_τ let $K^+(\xi)\subset\mathbb{R}^d_x\times\bar{\mathbb{R}}^+$ be a forward propagation cone and $K^-(\xi)=-K^+(\xi)$ be a backward propagation cone. Let

$$\Omega^\pm=\{(x,\xi)\colon x\notin\pi_xK^\pm(\xi)\} \tag{2.21}$$

where π_x is x-projection.

Then $\Omega^\pm$ are open sets and since $\pi_x K^+(\xi)\cap \pi_x K^-(\xi)=\{0\}$ we conclude that $\Omega^+\cup\Omega^-\supset \mathbb{S}^{d-1}\times\mathcal{W}$. We can then find smooth positively homogeneous of degree 0 with respect to x symbols $q^\pm(x,\xi)$ supported in $\Omega^\pm$ such that $q^++q^-=1$ on $\mathbb{S}^{d-1}\times\mathcal{W}$. Let $q^0=1-(q^++q^-)$; then $(A^0-\tau)$ is elliptic on $\operatorname{supp}(q^0)$.

Finally, let $Q^\pm$ and Q^0 be operators with the symbols $q^\pm(x,\xi)\phi_R(x)$ and $q^0(x|,\xi)\phi_R(x)$ correspondingly, where $\phi\in\mathscr{C}_0^\infty(\mathbb{R}^d\setminus 0)$, equal 1 as $c^{-1}\le |x|\le c$ with large enough constant c. Then

$$Q^++Q^-+Q^0=\phi_R(x), \tag{2.22}$$

where (2.18) holds and $(A-\tau)$ is elliptic on the support of the symbol of Q^0.

Then Proposition 2.4 below implies that for $R\le\varepsilon T$ with sufficiently small constant ε both (2.19) and (2.20) hold. On the other hand, ellipticity of $(A-\tau)$ on $\operatorname{supp}(Q^0)$ implies that

$$\|\varphi_\varepsilon(A-\lambda)(1-\psi_{R/2})Q^0\|\le C_s(h/R)^s. \tag{2.23}$$

Then we can make an induction step by n and to prove (2.15). After this, let us replace in (2.15) R and T by r and t. Next, for given R,T such that $R\le\varepsilon^3T$ let us plug into (2.15) $n=(T/R)^{\frac13}$, $t=T^{\frac23}R^{\frac13}=T/n$ and $r=T^{\frac13}R^{\frac23}=nR$ (obviously $r\le\varepsilon t$). We arrive to (2.14) with a different but still arbitrarily large exponent s. $\square$

As mentioned, we need the following proposition:

Proposition 2.4. *Let conditions of Theorem 1.1 be fulfilled. Let $\bar x\in\mathbb{R}^d\setminus 0$, $\bar\xi\in\mathcal{W}$ and assume that $0\notin \bar x+\pi_xK^\mp(\xi)$. Let $\mathcal{K}^\mp$ be a conical η-vicinity of $K^\mp(\xi)$ and $\mathcal{V}$ be ηR-vicinity of $\bar x$, $R=|x|$. Then*

$$\|Q'e^{\pm ih^{-1}TA}Q\|\le C_s(h/R)^s \tag{2.24}$$

provided $Q=Q(x,hD)$ and $Q'=Q'(x,hD)$ are operators with the symbols satisfying

$$|D_\xi^\alpha D_x^\beta Q|\le c_{\alpha\beta}r^{-|\beta|} \tag{2.25}$$

with $r=T+R$ and $r=R$ respectively, $R\ge R(\eta)$ and support of symbol of Q does not intersect with $\mathcal{V}+\mathcal{K}^\mp|_{t=T}$, symbol of Q' is supported in the sufficiently small vicinity of $(\bar x,\bar\xi)$.

Proof. Considering propagation in the zone $\{x\colon |x| \asymp r\}$, we see that the propagation speed with respect to ξ does not exceed $Cr^{-1-\delta}$. To prove this we scale $x \mapsto xr^{-1}$, $t \mapsto tr^{-1}$, $h \mapsto \hbar = hr^{-1}$ and apply the standard energy method (see Chapter 2 of [Ivr1]). We leave the easy details to the reader.

Therefore for time $t \asymp r$ variation of ξ does not exceed $Cr^{-\delta}$. Then, the propagation speed with respect to $\langle x, \ell(\bar{\xi})\rangle$ (which increases) is of magnitude 1 (as long as ξ remains in the small vicinity of $\bar{\xi}$). Again, to prove it we scale and apply the energy method (see Chapter 2 of [Ivr1]).

But then the contribution of the time interval $t \asymp r$ to the variation of ξ does not exceed $Cr^{-\delta}$ and therefore the variation of ξ for a time interval $[0, T]$ with $T \geq 0$ does not exceed $CR^{-\delta} \leq \eta$ for $R \geq R(\eta)$. □

Proposition 2.5. *In the framework of Theorem 1.1*

$$\|\psi_R e^{ih^{-1}TA}\varphi_\varepsilon(A-\lambda)\psi_R\| \leq C_s h^s, \tag{2.26}$$

provided $T \geq C_0 R$, $R \geq 1$.

Proof. It follows immediately from Proposition 2.4 with the semiclassical parameter hr^{-1} and with r set to its minimal value along the cone of propagation, which is 1. □

Combining Propositions 2.3 and 2.5 we arrive to

Corollary 2.6. *In the framework of Theorem 1.1*

$$\|\psi_R e^{ih^{-1}TA}\varphi_\varepsilon(A-\lambda)\psi_R\| \leq C_s h^s R^s T^{-s} \tag{2.27}$$

provided $T \geq C_0 R$, $R \geq 1$.

2.3 Traces and the End of the Proof

Proposition 2.7. *In the framework of Theorem 1.1 the following estimates hold for* $T \geq 1$

$$|F_{t\to\tau}\chi_T(t)u(x,x,t)| \leq C_s h^s (|x|+1)^{s+1}((|x|+1)+T)^{-s}, \tag{2.28}$$

$$|F_{t\to\tau}\chi_T(t)\int \psi_R(x)u(x,x,t)\,dx| \leq C_s h^s T^{-s}, \tag{2.29}$$

provided $\psi \in \mathscr{C}_0^\infty(B(0,1))$. *Further,*

$$|F_{t\to\tau}\chi_T(t)\int \psi_R(x)u(x,x,t)\,dx| \le C_s h^s R^{-s}T^{-s}, \tag{2.30}$$

provided $\psi \in \mathscr{C}_0^\infty(B(0,1)\setminus B(0,\frac{1}{2})$.

Proof. Estimate (2.28) follows immediately from (2.26). Estimate (2.30) follows from (2.26) and

$$|F_{t\to\tau}\chi_T(t)\int \psi_R(x)u(x,x,t)\,dx| \le C_s h^s R^{-s}T,$$

which holds because we can chose the time direction on the partition element (see Chapter 4 of [Ivr1]) and we chose the one in which $|x|\gtrsim R$ (which is possible; see the part of proof of Proposition 2.3 dealing with $Q^\pm$ and Q^0).

Finally, estimate (2.29) follows from (2.30). □

Then we immediately arrive to the following theorem, which in turn implies Theorem 1.1:

Theorem 2.8. *In the framework of Theorem 1.1 the following estimates hold*

$$|\partial_\tau^k\Bigl(e(x,x,\tau)-\sum_{n\le N-1}\kappa_n(x,\tau)h^{-d+n}\Bigr)| \le C_N h^{-d+N}(|x|+1)^{-N} + C_s h^s(|x|+1)^k \tag{2.31}$$

and for $\psi \in \mathscr{C}_0^\infty(B(0,1))$

$$|\partial_\tau^k\int\Bigl(e(x,x,\tau)-\sum_{n\le N-1}\kappa_n(x,\tau)h^{-d+n}\Bigr)\psi_R(x)\,dx| \le C_N h^{-d+N}. \tag{2.32}$$

2.4 Discussion

Corollary 2.9. *Let conditions of Theorem 1.1 be fulfilled. Assume that*

$$|D_x^\alpha V| \le c_\alpha(|\xi|+1)^m(|x|+1)^{-d-|\alpha|-\delta}. \tag{2.33}$$

Then the asymptotics of the Birman-Schwinger spectral shift function

$$\mathsf{N}_h(\tau) := \int\Bigl(e_h(x,x,\tau)-e_h^0(x,x,\tau)\Bigr)\,dx \sim \sum_{n\ge 0}\varkappa h^{-d+n} \tag{2.34}$$

is infinitely differentiable with respect to τ*. Here* $e_h^0(x,x,\tau)=\kappa_0^0 h^{-d}$ *and* $e_h^0(x,y,\tau)$ *is the Schwartz kernel of spectral projector for* $A^0(hD)$*, and*

$$\varkappa_n(\tau)=\int \bigl(\kappa_n(x,\tau)-\delta_{n0}\kappa^0\bigr)\,dx. \tag{2.35}$$

Indeed, condition (2.33) guarantees the absolute convergence of integrals in (2.35).

Remark 2.10. Our results could be easily generalized to non-semi-bounded elliptic A^0 (like in Subsection 3.1 of [Ivr3]). Then instead of $e(x,y,\lambda)$ one needs to consider $e(x,y,\lambda,\lambda')$ the Schwartz kernel of $\theta(\lambda-A)-\theta(\lambda'-A)$ and either impose conditions for both λ and λ', or only for λ and mollify with respect to λ'.

It looks strange that the last term in the remainder estimate (2.31) increases as $|x|$ increases, but so far I can neither improve it to the uniform with respect to x in the general case, nor show by the counter-example that such improvement is impossible. However I hope to prove

Conjecture 2.11. *Assume in addition that* A^0 *is a scalar operator and* $\Sigma_\lambda^0=\{\xi\colon A^0(\xi)=\lambda\}$ *is a* strongly convex surface *i.e.*

$$\pm\sum_{j,k} A^0_{\xi_j\xi_k}(\xi)\eta_j\eta_k\ge \epsilon|\eta|^2\qquad \forall\xi\in\Sigma^0_\lambda\ \ \forall\eta\colon \sum_j A^0_{\xi_j}(\xi)\eta_j=0, \tag{2.36}$$

where the sign depends on the connected component of Σ_λ*, containing* ξ*.*

Then the last term in the right-hand expression of (2.31) *could be replaced by* $C_s h^s(|x|+1)^{k-d}$*.*

Rationale here is that only few Hamiltonian trajectories from x with $|x|=R\gg 1$ pass close to the origin and even they do not spend much time there.

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Bethe-Sommerfeld Conjecture in Semiclassical Settings *,†

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Abstract

Under certain assumptions (including $d \geq 2$) we prove that the spectrum of a scalar operator in $\mathscr{L}^2(\mathbb{R}^d)$

$$A_\varepsilon(x, hD) = A^0(hD) + \varepsilon B(x, hD),$$

covers interval $(\tau - \epsilon, \tau + \epsilon)$, where A^0 is an elliptic operator and $B(x, hD)$ is a periodic perturbation, $\varepsilon = O(h^\varkappa)$, $\varkappa > 0$.

Further, we consider generalizations.

1 Introduction

1.1 Preliminary Remarks

This work is inspired by a paper [PS3] by L. Parnovski and A. Sobolev, in which a classical Bethe-Sommerfeld conjecture was proven for operators $(-\Delta)^m + B(x, D)$ with operator B of order $< 2m$. In this paper the crucial role was played by a (pseudodifferential) gauge transformation and thorough analysis of the resonant set, both introduced in the papers of L. Parnovski and R. Shterenberg [PSh1, PSh2, PSh3], S. Morozov, L. Parnovski and R. Shterenberg [MPS] and earlier papers by A. Sobolev [So2, So2], devoted to complete asymptotics of the integrated density of states.

Later in [Ivr3] I used the gauge same transformation in the semiclassical settings, which allowed me to generalize the results and simplify the proofs

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of those papers[1]. Now I would like to apply this gauge transform to Bethe-Sommerfeld conjecture in the semiclassical settings. The results obtained are more general (except the smoothness with respect to ξ assumptions in [PS3] are more general than here) and the proofs are simpler.

Consider a scalar self-adjoint h-pseudo-differential operator $A_h := A(x, hD)$ in $\mathbb{R}^d$ with the Weyl symbol $A(x,\xi)$, such that[2]

$$|D_x^\alpha D_\xi^\beta A(x,\xi)| \le c_{\alpha\beta}(|\xi|+1)^m \qquad \forall \alpha,\beta \tag{1.1}$$

and

$$A(x,\xi) \ge c_0|\xi|^m - C_0 \qquad \forall (x,\xi)\in\mathbb{R}^{2d}. \tag{1.2}$$

Then A_h is semibounded from below. Also we assume that it is Γ-periodic with the *lattice of periods* Γ:

$$A(x+\mathsf{y},\xi) = A(x,\xi) \qquad \forall x\in\mathbb{R}^n \quad \forall \mathsf{y}\in\Gamma. \tag{1.3}$$

We assume that Γ is non-degenerate[3] and denote by Γ^* the *dual lattice*:

$$\gamma\in\Gamma^* \iff \langle\gamma,\mathsf{y}\rangle\in 2\pi\mathbb{Z} \quad \forall \mathsf{y}\in\Gamma; \tag{1.4}$$

since we use Γ^* and it's elements in the paper much more often, than Γ and it's elements, it is more convenient for us to reserve notation γ for elements of Γ^*.

Also let $\mathcal{O} = \mathbb{R}^d/\Gamma$ and $\mathcal{O}^* = \mathbb{R}^d/\Gamma^*$ be *fundamental domains*; we identify them with domains in $\mathbb{R}^d$.

It is well-known that $\mathsf{Spec}(A)$ has a *band-structure*. Namely, consider in $\mathscr{L}^2(\mathcal{O})$ operator $A_h(\xi) = A(x,hD)$ with the *quasi-periodic boundary condition*:

$$u(x+\mathsf{y}) = e^{i\langle \mathsf{y},\xi\rangle}u(x) \qquad \forall x\in\mathcal{O} \quad \forall \mathsf{y}\in\Gamma \tag{1.5}$$

with $\xi\in\mathcal{O}^*$; it is called a *quasimomentum*. Then $\mathsf{Spec}(A_h(\xi))$ is discrete

$$\mathsf{Spec}(A_h(\xi)) = \bigcup_n \lambda_{n,h}(\xi) \tag{1.6}$$

---

[1] The other components of the proof were not only completely different, but in the framework of the different paradigm.

[2] In fact, we consider $A_h := A(x, hD, h)$.

[3] I.e. with the $\Gamma = \{\mathsf{y} = n_1\mathsf{y}_1 + \ldots + n_d\mathsf{y}_d,\ (n_1,\ldots,n_d)\in\mathbb{Z}^d\}$ with linearly independent $\mathsf{y}_1,\ldots,\mathsf{y}_d\in\mathbb{R}^d$.

and depends on ξ continuously. Further,

$$\operatorname{Spec}(A_h) = \bigcup_{\xi\in\mathcal{O}^*} \operatorname{Spec}(A_h(\xi)) =: \bigcup_n \Lambda_{n,h}, \tag{1.7}$$

with the *spectral bands* $\Lambda_{n,h} := \bigcup_{\xi\in\mathcal{O}^*}\{\lambda_{n,h}(\xi)\}$.

One can prove that the with of the spectral band near energy level τ is $O(h)$. Spectral bands could overlap but they also could leave uncovered intervals, called *spectral gaps*. It follows from [Ivr3] that in our assumptions (see below) the width of the spectral gaps near energy level τ is $O(h^\infty)$. Bethe-Sommerfeld conjecture in the semiclassical settings claims that there are no spectral gaps near energy level τ (in the corresponding assumptions, which include $d \ge 2$).

1.2 Main Theorem (Statement)

We assume that

$$A_h := A(x, hD) = A^0(hD) + \varepsilon B(x, hD), \tag{1.8}$$

where $A^0(\xi)$ satisfies (1.1), (1.2) and $B(x,\xi)$ satisfies (1.1) and (1.3) and $\varepsilon > 0$ is a small parameter. For $A^0(\xi)$ instead of $\lambda_n(\xi)$ we have

$$\lambda^0_\gamma(\xi) := A^0(h(\gamma+\xi)) \qquad \text{with} \ \ \gamma \in \Gamma^*. \tag{1.9}$$

Recall that (as in [Ivr3])

$$B(x,\xi) = \sum_{\gamma\in\Gamma} b_\gamma(\xi) e^{i\langle\gamma,x\rangle} \tag{1.10}$$

with $\Theta = \Gamma^*$ where due to (1.1)

$$|D_\xi^\beta b_\gamma(\xi)| \le C_{L\beta}(|\gamma|+1)^{-L}(|\xi|+1)^m \qquad \forall\beta \quad \forall(x,\xi)\in\mathbb{R}^{2d} \tag{1.11}$$

with an arbitrarily large exponent L.

Theorem 1.1. *Let $d \ge 2$ and let operator A_h be given by* (1.8) *with $\varepsilon = O(h^\vartheta)$ with arbitrary $\varkappa > 0$ and with $A^0_h = A^0(hD)$ satisfying* (1.1), (1.2) *and $B(x,\xi)$ satisfying* (1.1) *and* (1.3).

Further, assume that the microhyperbolicity *and* strong convexity *conditions on the energy level* τ *are fulfilled:*

$$|A^0(\xi)-\tau| + |\nabla_\xi A^0(\xi)| \ge \epsilon_0 \tag{1.12}$$

and

$$\pm\sum_{j,k} A^0_{\xi_j\xi_k}(\xi)\eta_j\eta_k \ge \epsilon_0|\eta|^2 \qquad \forall\xi\colon A^0(\xi)=\tau \quad \forall\eta\colon \sum_j A^0_{\xi_j}(\xi)\eta_j = 0. \tag{1.13}$$

Furthermore, assume that there exists $\xi\in\Sigma_\tau$ *such that for every* $\eta\in\Sigma_\tau$, $\eta\ne\xi$, *such that* $\nabla_\eta A^0(\eta)$ *is parallel to* $\nabla_\xi A^0(\xi)$ [4)]

(1.14) Σ_τ, *intersected with some vicinity of* η *and shifted by* $(\xi-\eta)$, *coincides in the vicinity of* ξ *with* $\{\zeta\colon \zeta_k = g(\zeta_{\hat k}\}$ *and* Σ_τ *coincides in the vicinity of* ξ *with* $\{\zeta\colon \zeta_k = f(\zeta_{\hat k}\}$ [5)] *and* $\nabla^\alpha(f-g)(0)\ne 0$ *for some* $\alpha\colon |\alpha|=2$ [6)].

Then $\operatorname{Spec}(A_h)\supset[\tau-\epsilon,\tau+\epsilon]$ *for sufficiently small* $\epsilon>0$.

Remark 1.2. (i) If Σ_τ is strongly convex and connected then for every $\xi\in\Sigma_\tau$ there exists exactly one antipodal point $\eta\in\Sigma_\tau$; then $\nu<0$ and assumption (1.14) is fulfilled. In particular, if $A^0(\xi)=|\xi|^m$, then $\eta=-\xi$ and $\nu=-1$.

(ii) If Σ_τ is is strongly convex and consists of p connected components, then the set $\mathfrak{Z}(\xi)=\{\eta\in\Sigma_\tau,\eta\ne\xi\colon \nabla_\eta A^0(\eta)\parallel\nabla_\xi A^0(\xi)\}$ contains exactly $2p-1$ elements, and for p of them $\nu<0$ and assumption (1.14) is fulfilled for sure, while for $(p-1)$ of them $\nu>0$.

1.3 Idea of the Proof and the Plan of the Paper

One needs to understand, how gaps could appear, why they appear if $d=1$ and why it is not the case if $d\ge 2$. Observe that $\lambda_n(\xi)$ can be identified with some $\lambda^0_\gamma(\xi)$ only locally, if $\lambda^0_\gamma(\xi)$ is sufficiently different from $\lambda^0_{\gamma'}(\xi)$ for any $\gamma'\ne\gamma$.

---

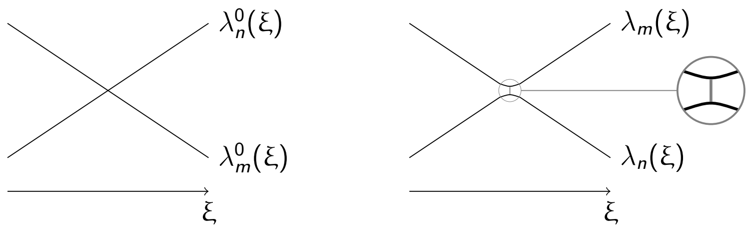
4) I.e. $\eta A^0(\eta)=\nu\nabla_\xi A^0(\xi)$ with $\nu\ne 0$; we call η *antipodal point.*

5) With $\zeta_{\hat k}$ meaning all coordinates except ζ_k.

6) Obviously $\nabla(f-g)(0)=0$. One can prove easily, that if this condition holds at ξ with some $\alpha\colon |\alpha|>2$, then changing slightly ξ, we make it fulfilled with $|\alpha|=2$.

Indeed, in the basis of eigenfunctions of $A^0_\xi(hD)$ [7] perturbation $\varepsilon B(x,hD)$ can contain out-of-diagonal elements $\varepsilon b_{\gamma-\gamma'}(\xi)$ and such identification is possible only if $|\lambda^0_\gamma(\xi)-\lambda^0_{\gamma'}(\xi)|$ is larger than the size of such element.

If $d=1$, $A^0(\xi)=\xi^2$ and $\varepsilon\le\epsilon' h$ with sufficiently small $\epsilon'>0$ and $\tau\asymp 1$, it can happen only if γ' coincides with $-\gamma$ or with one of two adjacent points in Γ^* and $|\xi-\frac{1}{2}(\gamma+\gamma')|=O(\varepsilon h^\infty)$. This exclude from possible values of either $\lambda^0_\gamma(\xi)$ or $\lambda^0_{\gamma'}(\xi)$ the interval of the width $O(\varepsilon h^\infty)$ and on such interval can happen (and really happens for a generic perturbation) the realignment:



(a) (b)

Figure 1: Spectral gap is a gray interval

If $d\ge 2$ the picture becomes more complicated: there are much more opportunities for $\lambda^0_\gamma(\xi)$ and $\lambda^0_{\gamma'}(\xi)$ to become close, even if γ and γ' are not that far away; on the other hand, there is a much more opportunities for us to select $\xi=h(\gamma+\xi)\in\Sigma_\tau$ and then to adjust ξ so that $\xi=h(\gamma+\xi)$ remains on Σ_τ but $\eta=h(\gamma'+\xi)$ moves away from Σ_τ sufficiently far away[8] and then tune-up ξ once again so that $\tau\in\operatorname{Spec}(A_h(\xi))$.

In fact, we prove the following statement which together with Theorem 1.1 (which follows from it trivially) are semiclassical analogue of Theorem 2.1 of [PS3]:

Theorem 1.3. *In the framework of Theorem 1.1 there exist n and ξ^* such that $\lambda_n(\xi^*)=\tau$ and $\lambda_n(\xi)$ covers interval $[\tau-\upsilon h,\tau+\upsilon h]$ when ξ runs ball $\mathsf{B}(\xi^*,\upsilon)$ while $|\lambda_m(\xi)-\tau|\ge\epsilon\upsilon h$ for all $m\ne n$ and $\xi\in\mathsf{B}(\xi^*,\upsilon)$. Here*

$$\upsilon=\epsilon\begin{cases} h^{(d-1)^2}\min(1,\ \varepsilon^{-3(d-1)/2}h^{(d-1)+\sigma}) & d\ge 3,\\ h\min(|\log h|^{-1},\ \varepsilon^{-3/2}h^\sigma) & d=2\end{cases}\tag{1.15}$$

[7] Consisting of $\exp(i\langle x,\gamma+\xi\rangle)$.

[8] This will happen if either $\nabla_\eta A^0(\eta)$ differs from $\nu\nabla_\xi A^0(\xi)$, or if coincides with it but (1.14) is fulfilled.

with arbitrarily small exponent $\sigma > 0$*.*

Proof of Theorem 1.3 occupies two next sections. In Section 2 we reduce operator in the vicinity of Σ_τ to the block-diagonal form and study its structure. To do this we need to examine the structure of the resonant set of the operator. In Section 3 we prove Theorem 1.3 and thus Theorem 1.1.

Finally, in Section 4 we discuss our results and the possible improvements.

2 Reduction of Operator

2.1 Reduction

On this step we reduce A to the block-diagonal form in the vicinity of Σ_τ

$$\Omega_\tau := \{\xi\colon |A^0(\xi) - \tau| \le C\varepsilon h^{-\delta}\}. \tag{2.1}$$

In what follows, we assume that $\varepsilon \ge h$, i.e.

$$h \le \varepsilon \le h^{\vartheta}, \qquad \vartheta > 0. \tag{2.2}$$

To do this we need just to repeat with the obvious modifications definitions and arguments of Sections 1 and 2 of [Ivr3]. Namely, now $\Theta := \Gamma^*$ is a non-degenerate lattice rather than the pseudo-lattice, as it was in that paper, and all conditions 1.2, 1.3, 1.5, 1.6, and 3.3, are fulfilled with $\Theta' := \Theta \cap \mathsf{B}(0,\omega)$ with $\omega = h^{-\varkappa}$ where we select sufficiently small $\varkappa > 0$ later and $\Theta'_K = \Theta \cap \mathsf{B}(0, K\omega)$ be an arithmetic sum of K copies of Θ' with sufficiently large K to be chosen later.

We call point ξ *non-resonant* if

$$|\langle \nabla_\xi A^0(\xi), \theta\rangle| \ge \rho \qquad \forall \theta \in \Theta'_K \setminus 0 \tag{2.3}$$

with $\rho \in [\varepsilon^{1/2}h^{-\delta}, h^{\delta}]$ with arbitrarily small $\delta > 0$. Otherwise we call it *resonant*. More precisely

$$\Lambda := \bigcup_{\theta\in\Theta'_K\setminus 0} \Lambda(\theta), \tag{2.4}$$

where $\Lambda(\theta)$ is the set of ξ, violating (2.3) for given $\theta \in \Theta'_K \setminus 0$.

It obviously follows from the microhyperbolicity and strong convexity assumptions (1.12) and (1.13) that

(2.5) $\upmu_\tau$-measure[9] of $\Lambda\cap\Sigma_\tau$, does not exceed $C_0 r^{d-1}\rho$ and Euclidean measure of $\Lambda\cap\{\xi\colon |A^0(\xi)-\tau|\le\varsigma\}$ does not exceed $C_0 r^{d-1}\rho\varsigma$, where $r=Kh^{-\varkappa}$.

Indeed, $(d-1)$-dimensional measure of $\{x\colon |x|=1,\ |\langle x,\theta\rangle|\le\rho\}$ does not exceed $C_0|\theta|^{-1}\rho$ and and due to microhyperbolicity and strong convexity assumptions maps $\Sigma_\tau\to\nabla A^0(\xi)/|\nabla A^0(\xi)|\in\mathbb{S}^{d-1}$ and

$$\{\xi\colon |A^0(\xi)-\tau|\le\varsigma\}\to(\nabla A^0(\xi)/|\nabla A^0(\xi)|, A^0(\xi))\in\mathbb{R}^d$$

are diffeomorphisms.

Furthermore, according to Proposition 2.7 of [Ivr3] that on the non-resonant set one can "almost" diagonalize $A(x,hD)$. More precisely

Proposition 2.1. *Let assumptions* (1.12) *and* (1.13) *be fulfilled.*

(i) Then there exists a periodic pseudodifferential operator $P=P(x,hD)$ such that

$$\bigl(e^{-i\varepsilon h^{-1}P}Ae^{i\varepsilon h^{-1}P}-\mathcal{A}\bigr)Q\equiv 0 \tag{2.6}$$

with

$$\mathcal{A}=A^0(hD)+\varepsilon B'(hD)+\varepsilon B''(x,hD) \tag{2.7}$$

modulo operator from $\mathscr{H}^m$ to $\mathscr{L}^2$ with the operator norm $O(h^M)$ with M arbitrarily large and $K=K(M,d,\delta)$ in the definition of non-resonant point provided $Q=Q(hD)$ has a symbol, supported in $\{\xi\colon |A^0(\xi)-\tau|\le 2\varepsilon h^{-\delta}\}$.

Here $P(x,hD)$, $B'(hD)$ and $B''(x,hD)$ are operator with Weyl symbols of the same form (1.10) *albeit such that*

$$|D_\xi^\alpha D_x^\beta P|\le c_{\alpha\beta}\rho^{-1-|\alpha|}\qquad\forall\alpha,\beta, \tag{2.8}$$

$$|D_\xi^\alpha D_x^\beta B''|\le c'_{\alpha\beta}\rho^{-|\alpha|}\qquad\forall\alpha,\beta, \tag{2.9}$$

and symbol of B' also satisfies (2.9)*.*

(ii) Further,

$$\xi\notin\Lambda(\theta)\implies b''_\theta(\xi)=0. \tag{2.10}$$

and $B'(\xi)$ coincides with $b_0(\xi)$ modulo $O(\varepsilon\rho^{-2})$.

[9] $\upmu_\tau=d\xi : dA^0(\xi)$ is a natural measure on Σ_τ.

In what follows

$$\mathcal{A}^0(hD) := A^0(hD) + \varepsilon B'(hD) \qquad \text{and} \qquad \mathcal{B} := B''(x, hD). \tag{2.11}$$

Remark 2.2. (i) Eigenvalues of $\mathcal{A}^0$ are

$$\lambda_\gamma(\xi) = \mathcal{A}^0(h(\gamma + \xi)). \tag{2.12}$$

(ii) If $\xi = h(\gamma + \xi)$ is non-resonant, then due to (2.10) in $\epsilon'\rho$-vicinity of ξ this $\lambda_\gamma(\xi)$ is also an eigenvalue of $\mathcal{A}$.

(iii) Without any loss of the generality one can assume that

$$|\theta| \ge \varepsilon h^{-\delta} \implies b''_\theta = 0. \tag{2.13}$$

We assume that this is the case.

(iv) Let us replace operator $\mathcal{A}$ defined by (2.7) by operator

$$\mathcal{A}' = \mathcal{A}^0(hD) + \varepsilon\mathcal{B}'(x, hD), \qquad \mathcal{B}'(x, hD) = T(hD)\mathcal{B}T(hD) \tag{2.14}$$

with $T(hD)$ operator with symbol $T(\xi)$ which is a characteristic function of Ω_τ defined by (2.1) with $C = 6$. Then (2.6) holds.

From now on $\mathcal{A} := \mathcal{A}'$ and $\mathcal{B} := \mathcal{B}'$.

It would be sufficient to prove Theorem 1.3 for operator $\mathcal{A}$. Indeed,

Proposition 2.3. *(i) For each point* $\lambda \in \operatorname{Spec}(A(\xi)) \cap \{|\lambda - \tau| \le \varepsilon h^{-\delta}\}$ $\operatorname{dist}(\lambda, \operatorname{Spec}(\mathcal{A}(\xi)) \le Ch^M$.

(ii) Conversely, for each point $\lambda \in \operatorname{Spec}(\mathcal{A}(\xi)) \cap \{|\lambda - \tau| \le \varepsilon h^{-\delta}\}$ $\operatorname{dist}(\lambda, \operatorname{Spec}(A(\xi)) \le Ch^M$.

(iii) Furthermore, if $\lambda \in \operatorname{Spec}(A(\xi)) \cap \{|\lambda - \tau| \le \varepsilon h^{-\delta}\}$ *is a simple eigenvalue separated from the rest of* $\operatorname{Spec}(A(\xi))$ *by a distance at least* $2h^{M-1}$*, then there exists* $\lambda' \in \operatorname{Spec}(\mathcal{A}(\xi)) \cap \{|\lambda' - \lambda| \le Ch^M\}$ *separated from the rest of* $\operatorname{Spec}(\mathcal{A}(\xi))$ *by a distance at least* h^{M-1}.

(iv) Conversely, if $\lambda' \in \operatorname{Spec}(\mathcal{A}(\xi)) \cap \{|\lambda - \tau| \le \varepsilon h^{-\delta}\}$ *is a simple eigenvalue separated from the rest of* $\operatorname{Spec}(\mathcal{A}(\xi))$ *by a distance at least* $2h^{M-1}$*, then there exists* $\lambda \in \operatorname{Spec}(A(\xi)) \cap \{|\lambda' - \lambda| \le Ch^M\}$ *separated from the rest of* $\operatorname{Spec}(A(\xi))$ *by a distance at least* h^{M-1}.

Proof. Trivial proof is left to the reader. □

Remark 2.4. One can generalize Statements (iii) and (iv) of Proposition 2.3 from simple eigenvalues to subsets of $\mathsf{Spec}(A(\xi))$ and $\mathsf{Spec}(\mathcal{A}(\xi))$ separated by the rest of the spectra; these subsets will contain the same number of elements.

2.2 Classification of Resonant Points

We start from the case $d = 2$. Then we have only one kind of resonant points $\Xi_1 = \Lambda$. If $d \geq 3$ then there are $(d-1)$ kinds of resonant points. First, following [PS3] consider *lattice spaces* $\mathfrak{V}$ spanned by n linearly independent elements $\theta_1, \dots, \theta_n \in \Gamma^* \cap \mathsf{B}(0, r)$, where we take $r = Kh^{-\varkappa}$. Let $\mathcal{V}_n$ be the set of all such spaces.

It is known [PS3] that

Proposition 2.5. *For $\mathfrak{V} \in \mathcal{V}_n$, $\mathfrak{W} \in \mathcal{V}_m$ either $\mathfrak{V} \subset \mathfrak{W}$, or $\mathfrak{W} \subset \mathfrak{V}$ or the angle*[10] *between $\mathfrak{V}$ and $\mathfrak{W}$ is at least ϵr^{-L} with $L = L(d)$ and $\epsilon = \epsilon(d, \Gamma)$.*

Fix $0 < \delta_1 < \dots < \delta_n$ arbitrarily small and for $\mathfrak{V} \in \mathcal{V}_n$ let us introduce

$$\Lambda(\mathfrak{V}, \rho_n) \coloneqq \{\xi \in \Omega_\tau \colon |\langle \nabla_\xi A^0(\xi), \theta\rangle| \leq \rho_n |\theta| \quad \forall \theta \in \mathfrak{V}\} \tag{2.15}$$

with $\rho_n = \varepsilon^{\frac{1}{2}} h^{-\delta_n}$.

We define Ξ_n by induction. First, $\Xi_d = \emptyset$. Assume that we defined $\Xi_d, \dots, \Xi_{n+1}$. Then we define

$$\Xi_n \coloneqq \bigcup_{\mathfrak{V} \in \mathcal{V}_n,\ \xi \in \Lambda(\mathfrak{V}) \cap \Omega_\tau} (\xi + \mathfrak{V}) \cap \Omega_\tau. \tag{2.16}$$

It follows from Proposition 2.5 that

Proposition 2.6. *Let $\varkappa > 0$ in the definition of Θ' and $\delta > 0$ in the definition of Ω_τ be sufficiently small*[11]*. Then for sufficiently small h*

(i) $\Xi_n \subset \bigcup_{\mathfrak{V} \in \mathcal{V}} \Lambda(\mathfrak{V}, 2\rho_n)$.

[10] This angle $\widehat{(\mathfrak{V}, \mathfrak{W})}$ is defined as the smallest possible angle between two vectors $v \in \mathfrak{V} \ominus (\mathfrak{V} \cap \mathfrak{W})$ and $w \in \mathfrak{W} \ominus (\mathfrak{V} \cap \mathfrak{W})$.

[11] They depend on ϑ and $\delta_1, \dots, \delta_n$.

(ii) If $\xi\notin\Xi_{n+1}$ and $\xi\in\xi'+\mathfrak{V}$, $\xi\in\xi''+\mathfrak{W}$ for $\xi'\in\Lambda(\mathfrak{V})$, $\xi''\in\Lambda(\mathfrak{W})$ with $\mathfrak{V},\mathfrak{W}\in\mathcal{V}_n$, then $\mathfrak{V}=\mathfrak{W}$.

Corollary 2.7. *Let $\varkappa>0$ in the definition of Θ' and $\delta>0$ in the definition of Ω_τ be sufficiently small*[11]*. Let h be sufficiently small.*

Then for each $\xi\in\Xi_n\setminus\Xi_{n+1}$ is defined just one $\mathfrak{V}=\mathfrak{V}(\xi)$ such that $\xi\in\xi'+\mathfrak{V}$ for some $\xi'\in\Lambda(\mathfrak{V})$.

(2.17) We slightly change definition of Ξ_n: $\xi=h(\gamma+\xi)\in\Xi_{n,\mathsf{new}}$ iff $h\gamma\in\Xi_n$. From now on $\Xi_n\coloneqq\Xi_{n,\mathsf{new}}$.

Consider $\xi',\xi''\in\Xi_n\setminus\Xi_{n+1}$. We say that $\xi'\cong\xi''$ if there exists $\xi\in\mathfrak{V}$, $\mathfrak{V}\in\mathcal{V}$ such that $\xi',\xi''\in\xi+\mathfrak{V}$ and if $\xi'-\xi''\in\Gamma$. In virtue of above

(2.18) This relation is reflexive, symmetric and transitive.

For $\xi\in\Xi_n$ we define

$$\mathfrak{X}(\xi)=\{\xi':\,\xi'\cong\xi\}. \tag{2.19}$$

Then

$$\operatorname{diam}(\mathfrak{X}(\xi))\le C\rho_{d-1}. \tag{2.20}$$

2.3 Structure of Operator $\mathcal{A}$

For $\xi\in\Xi_n\setminus\Xi_{n+1}$ denote by $\mathfrak{H}(\xi)$ the subspace $\mathscr{L}^2(\mathcal{O})$ consisting of functions of the form

$$\sum_{\xi'\in\mathfrak{X}(\xi)} c_{\xi'}e^{i\langle x,\xi'\rangle}. \tag{2.21}$$

In virtue of the properties of $\mathcal{A}$ and $\mathcal{B}$ and of resonant sets we arrive to

Proposition 2.8. *Let $\varkappa>0$ in the definition of Θ' and $\delta>0$ in the definition of Ω_τ be sufficiently small*[11]*. Let h be sufficiently small.*

Then for $\xi\in\Xi_n\setminus\Xi_{n+1}$ operators $\mathcal{B}$ and $\mathcal{A}$ transform $\mathfrak{H}(\xi)$ into $\mathfrak{H}(\xi)$.

Let us denote by $\mathcal{A}_\gamma(\xi)$ and $\mathcal{B}_\gamma(\xi)$ restrictions of $\mathcal{A}$ and $\mathcal{B}$ to $\mathfrak{H}(h(\gamma+\xi))$. Here for $n=0$ we consider Ξ_0 to be the set of all non-resonant points and $\mathfrak{X}(\xi)=\{\xi\}$ for $\xi\in\Xi_0$.

Then due to Propositions 2.5 and 2.8 we arrive to

Proposition 2.9. *(i) For each point* $\lambda \in \mathsf{Spec}(A(\xi)) \cap \{|\lambda - \tau| \le \varepsilon h^{-\delta}\}$ *exists* $\gamma \in \Gamma^*$ *such that* $\xi = h(\gamma + \xi) \in \Omega_\tau$ *and* $\mathsf{dist}(\lambda, \mathsf{Spec}(\mathcal{A}_\gamma(\xi)) \le Ch^M$.

(ii) Conversely, for each point $\lambda \in \mathsf{Spec}(\mathcal{A}_\gamma(\xi)) \cap \{|\lambda - \tau| \le \varepsilon h^{-\delta}\}$ *and* $\xi = h(\xi + \gamma)$, $\mathsf{dist}(\lambda, \mathsf{Spec}(A(\xi)) \le Ch^M$.

(iii) Further, if $\lambda \in \mathsf{Spec}(A_\gamma(\xi)) \cap \{|\lambda - \tau| \le \varepsilon h^{-\delta}\}$ *is a simple eigenvalue separated from the rest of* $\mathsf{Spec}(A(\xi))$ *by a distance at least* $2h^{M-1}$*, then there exist* γ *and* λ'*, such that for* $\xi = h(\gamma+\xi)$, $\lambda' \in \mathsf{Spec}(\mathcal{A}(\xi)) \cap \{|\lambda' - \lambda| \le Ch^M\}$*, separated from the rest of* $\mathsf{Spec}(\mathcal{A}_\gamma(\xi))$ *by a distance at least* h^{M-1} *and from* $\bigcup_{\gamma' \in \Gamma^*,\ \gamma' \ne \gamma} \mathsf{Spec}(\mathcal{A}_{\gamma'}(\xi)$ *by a distance at least* h^{M-1} *as well.*

(iv) Conversely, if $\lambda' \in \mathsf{Spec}(\mathcal{A}_\gamma(\xi)) \cap \{|\lambda - \tau| \le \varepsilon h^{-\delta}\}$ *is a simple eigenvalue separated from the rest of* $\mathsf{Spec}(\mathcal{A}_\gamma(\xi))$ *by a distance at least* $2h^{M-1}$*, and also separated from* $\bigcup_{\gamma' \in \Gamma^*,\ \gamma' \ne \gamma} \mathsf{Spec}(\mathcal{A}_{\gamma'}(\xi))$ *by a distance at least* $2h^{M-1}$*, then there exists* $\lambda \in \mathsf{Spec}(A(\xi)) \cap \{|\lambda' - \lambda| \le Ch^M\}$ *separated from the rest of* $\mathsf{Spec}(A(\xi))$ *by a distance at least* h^{M-1}*.*

Proof. Proof is trivial. □

3 Proof of Theorem 1.3

3.1 Choosing γ^*

The first approximation is $\xi^* \in \Sigma_\tau$ satisfying (1.14). Any $\xi \in \Sigma_\tau$ in ϵ'-vicinity of ξ^* also fits provided $\epsilon' > 0$ is sufficiently small.

(3.1) One can select $\xi^*_{\mathsf{new}} \in \Sigma_\tau$ such that $|\xi^*_{\mathsf{new}} - \xi^*| \le h^\delta$ and ξ^*_{new} satisfies (1.14) with $\rho = \gamma := h^\delta$. Here $\delta > 0$ is arbitrarily small and $\varkappa = \varkappa(\delta)$.

Indeed, it follows from (2.5). From now on $\xi^* := \xi^*_{\mathsf{new}}$.

Then, according to Proposition 2.1 we can diagonalize operator in γ-vicinity of ξ^* and there $\rho = \gamma$. Then there

$$|\nabla^\alpha(\mathcal{A}^0 - A^0)| \le C_\alpha(\varepsilon + \varepsilon^2\rho^{-2-|\alpha|}) \tag{3.2}$$

and in particular

$$|\nabla^\alpha(\mathcal{A}^0 - A^0)| \le Ch^\delta \qquad \text{for} \quad |\alpha| \le 2. \tag{3.3}$$

Let

$$\Sigma'_\tau = \{\xi\colon \mathcal{A}^0(\xi) = \tau\}. \tag{3.4}$$

Then in the non-resonant points we are interested in functions $\lambda_\gamma(\xi) = \mathcal{A}^0(h(\gamma+\xi))$ rather than in $\lambda^0_\gamma(\xi) = A^0(h(\gamma+\xi))$. One can prove easily the following statements:

Proposition 3.1. *(i) One can select* $\xi^* := \xi^*_{\mathsf{new}} \in \Sigma'_\tau$ *satisfying* (1.14) *and non-resonant with* $\rho = \gamma$.

(ii) Further, all antipodal to ξ^* *points* $\xi^*_1, \dots, \xi^*_{2p-1}$ *have the same properties.*

Let $\xi^* =: h(\gamma^* + \xi^*)$, $\gamma^* \in \Gamma^*$ and $\xi^* \in \mathcal{O}^*$. Then values in the nearby points are sufficiently separated:

$$|\lambda_\gamma(\xi) - \lambda_{\gamma^*}(\xi)| \ge \epsilon h^{1+\delta} \qquad \forall \gamma\colon |\gamma - \gamma^*| \le Kh^{-\varkappa} \quad \forall \xi \in \mathcal{O}^*. \tag{3.5}$$

Indeed, $|\gamma - \gamma^*| \le Kh^{-\varkappa}$ implies that $(\gamma - \gamma^*) \in \Theta'_K$ and then

$$|\langle \nabla \mathcal{A}^0(\xi^*), \gamma - \gamma^*\rangle| \ge \gamma$$

while

$$|\lambda_\gamma(\xi) - \lambda_{\gamma^*}(\xi) - h\langle \nabla \mathcal{A}^0(\xi^*), \gamma - \gamma^*\rangle| \le Ch^{3-3\varkappa}.$$

3.2 Non-Resonant Points

Consider other non-resonant points (with $\rho = \varepsilon^{1/2}h^{-\delta}$). Let us determine how $\lambda_\gamma(\xi)$ changes when we change ξ. Due to (3.3)

$$\delta\lambda_\gamma := \lambda_\gamma(\xi + \delta\xi) - \lambda_\gamma(\xi) = h\langle \nabla A^0(\xi), \delta\xi\rangle + O(h^2|\delta\xi|^2). \tag{3.6}$$

To preserve $\lambda_{\gamma^*}(\xi) = \tau$ in the *linearized settings* we need to shift ξ by $\delta\xi$ which is orthogonal to $\nabla_\xi \mathcal{A}(\xi^*)$.

Let us take $\delta\xi = t\eta$

$$\ell\colon |\eta| = 1, \qquad \langle \nabla \mathcal{A}^0(\xi^*), \eta\rangle = 0. \tag{3.7}$$

Then in all non-resonant ξ the shift will be $\langle \nabla_\xi \mathcal{A}(\xi), \delta\xi\rangle$ with an absolute value $|\langle \nabla_\xi \mathcal{A}(\xi), \eta\rangle| \cdot |t|$.

Case $d=2$. Let us start from the easiest case $d=2$. Without any loss of the generality we assume that ξ^* is strictly inside $\mathcal{O}^*$ (at the distance at least $C\epsilon^*$ from the border). Then there is just one tangent direction η and

$$|\langle \nabla_\xi \mathcal{A}^0(\xi)|_{\xi=h\gamma}, \eta\rangle| \asymp |\sin\varphi(\gamma^*,\gamma)| \asymp h \min_{1\le k\le 2p} |\gamma-\gamma^*_k| \tag{3.8}$$

where $\varphi(\gamma^*,\gamma)$ is an angle between $\nabla_\xi \mathcal{A}^0(\xi)|_{\xi=h\gamma^*}$ and $\nabla_\xi \mathcal{A}^0(\xi)|_{\xi=h\gamma}$, and $\xi^*_1,\dots,\xi^*_{2p-1}$ are antipodal points, and $\xi^*_{2p}=\xi^*$.

As long as $\min_{1\le k\le 2p}|\gamma-\gamma^*_k| \gtrsim h^{1-\varkappa}$ we may replace here $\xi=h(\gamma+\xi)$ by $\xi=h\gamma$ and $\mathcal{A}^0$ by $\mathcal{A}$. In the nonlinear settings to ensure that

$$\lambda_{\gamma^*}(\xi^*+\delta\xi(t))=\tau \tag{3.9}$$

we need to include in $\delta\xi(t)$ a correction: $\delta\xi(t)=t\eta+O(t^2)$ but still

$$\frac{d}{dt}\lambda_\gamma(\xi^*+\delta\xi(t)) \asymp h\langle \nabla_\xi\mathcal{A}(\xi)|_{\xi=h\gamma},\eta\rangle^{-1}. \tag{3.10}$$

Then the set $\mathcal{T}(\xi) \coloneqq \{t\colon |t|\le\epsilon_0,\ |\mathcal{A}^0(\xi(t))-\tau|\le\upsilon h\}$ is an interval of the length $\asymp\upsilon$ and then the union of such sets over $\xi=h\gamma+\xi$ with indicated γ does not exceed $R\upsilon$ with

$$R\coloneqq \sum_\gamma |\langle\nabla_\xi\mathcal{A}(\xi)|_{\xi=h\gamma},\eta\rangle|^{-1}, \tag{3.11}$$

where we sum over set $\{\gamma\colon |\gamma-\gamma^*|\gtrsim h^{-\varkappa}\ \&\ |\lambda_\gamma(h\gamma)-\tau|\le 2Ch\}$. The last restriction is due to the fact that $\mathcal{T}(\xi)\ne\emptyset$ only for points with $|\lambda_\gamma(h\gamma)-\tau|\le 2Ch$.

One can see easily that $R\asymp h^{-1}|\log h|$. Then, as $R\upsilon\le\epsilon'$ the set $[-\epsilon_0,\epsilon_0]\setminus\bigcup_\gamma \mathcal{T}(h(\gamma+\xi))$ contains an interval of the length $\ell=\upsilon$ and for all t, belonging to this interval,

$$|\lambda_\gamma(h(\gamma+\xi+\delta\xi(t)))-\tau|\ge\epsilon\upsilon h. \tag{3.12}$$

Then we need to take $\upsilon=\epsilon R^{-1}=\epsilon h|\log h|^{-1}$ and for $d=2$ as far as non-resonant are concerned, Theorem 1.3 is almost proven[12)].

[12)] We need to cover almost antipodal points and it will be done in the end of this subsection. We need to consider resonant points and as well, and it will be done in the next subsection.

Case $d\ge 3$. In this case we need to be more subtle and to make $(d-1)$ steps. We start from the point $\xi^*=h(\gamma^*+\xi^*)$; again without any loss of the generality we assume that ξ^* is strictly inside $\mathcal{O}^*$ (at the distance at least $C\epsilon^*$ from the border). Then after each step below it still will be the case (with decreasing constant).

Step I. On the first step we select $\eta=\eta_1$ and consider only γ such that (3.8) holds; more precisely, the left-hand expression needs to be greater than the right-hand expression, multiplied by ϵ [13]. Then $R\asymp h^{1-d}$ and therefore exists ξ^* such that $\lambda_{\gamma^*}(\xi^*)=\tau$ and $|\lambda_\gamma(\xi^*)-\tau|\ge\epsilon\upsilon_1 h$ with $\upsilon_1=\epsilon h^{d-1}$ for all γ indicated above.

Step II. On the second step we select $\eta=\eta_2$ perpendicular to η_1. To preserve inequality (3.12) (with smaller constant ϵ) for γ, already covered by *Step I*, we need to take $|\delta\xi|\le\epsilon'\upsilon_1$ and consider $\delta\xi=t\eta_2+O(t^2)$.

Then the same arguments as before results in inequality (3.12) with $\upsilon:=\upsilon_2=\epsilon R^{-1}\upsilon_1$ for a new bunch of points. Then for $d=3$ as far as non-resonant are concerned, Theorem 1.3 is almost proven[13].

Next steps. Continuing this process, on k-th step we select η_k orthogonal to $\eta_1,\dots,\eta_{k-1}$. Then we get $\upsilon_k=\epsilon R^{-1}\upsilon_{k-1}$ and on the last $(d-1)$-th step we achieve a separation at least $\upsilon_{d-1}=\epsilon R^{1-d}$.

Remark 3.2. In Subsection 4.1 we discuss how to increase υ for $d\ge 3$.

Almost Antipodal Points. We need to cover points with $|\xi-\xi^*_k|\le h^{1-\kappa}$ for $k=1,\dots,2p-1$ and as we already know for each k (and fixed ξ) there exists no more than one such point $\xi=h(\gamma+\xi)$ with $|\lambda_\gamma(\xi)-\tau|\lesssim h^{1+\delta}$.

We take care of such points during *Step I*. Observe that during this step we automatically take care of any point with

$$|\nabla_\xi\mathcal{A}^0(\xi),\eta_1\rangle|\ge\epsilon h, \tag{3.13}$$

assuming that $|t|\le\epsilon_0$ with sufficiently small $\epsilon_0=\epsilon_0(\epsilon)$.

Let us select η_1 so that on η_1 quadratic forms at points $\xi^*_1,\dots,\xi^*_{2p-1}$ in condition (1.14) are different from one at point ξ^* by at least ϵ_0. Then for each $j=1,\dots,2p-1$ the the measure of the set

$$\{t\colon |t|\le\epsilon_0,\ |\lambda_{\gamma_j}(\xi+\delta\xi(t))|\le\upsilon h\}$$

[13] One can see easily, that the opposite inequality holds.

does not exceed $Ch^{-1}(\upsilon h)^{\frac{1}{2}}$, and then the measure of the union of such sets (by j) also does not exceed it and therefore for $\upsilon_1 = \epsilon_1 h^{d-1}$ (for $d \geq 3$) and $\upsilon_1 = \epsilon_1 h|\log h|^{-1}$ (for $d = 2$) with sufficiently small ϵ_1 we can find $t\colon |t| \leq \epsilon_0$ so that condition (3.8) is fulfilled for all non-resonant points.

3.3 Resonant Points

Next on this step we need to separate $\lambda_{\gamma^*}(\xi)$ from all $\lambda_n(\xi)$ (save one, coinciding with it) by the distance at least υh by choosing ξ. We can during the same steps as described in the previous section: let $\lambda_{\gamma,j}(\xi)$ denote eigenvalues of $\mathcal{A}_\gamma(\xi)$ with $j = \#\mathfrak{X}(\gamma h)$.

Observe that both $\mathcal{A}_\gamma(\xi)$ and $\#\mathfrak{X}(\gamma h)$ depend on the equivalency class $[\gamma]$ of γ rather than on γ itself and that

$$\sum_{[\gamma]} \#\mathfrak{X}(\gamma h) = \sum_{1\leq n\leq d-1} \#(\Xi_n) = O(h^{1-d+\sigma'} + \varepsilon^{3/2}h^{-d-\sigma}), \tag{3.14}$$

where on the left $[\gamma]$ runs over all equivalency classes with $\gamma \in \bigcup_{1\leq n\leq d-1} \Xi_n$.

We also observe that for resonant points

$$|\sin\varphi(\xi,\xi^*)| \geq \epsilon h^\delta \tag{3.15}$$

and therefore for λ'_γ, which are eigenvalues of $\mathcal{A}^0(h(\gamma+\xi))$ [14] (3.10) holds and signs are the same for γ in the same block. On the other hand,

$$|\frac{d}{dt}\mathcal{B}(h(\gamma+\xi^*+\delta\xi(t))| \leq C\varepsilon h \ll h^{1+\delta'} \tag{3.16}$$

and therefore for $\lambda_{\gamma,j}(t)$ which are eigenvalues of $\mathcal{A}_{[\gamma]}(\xi)$ (3.10) sill holds.

Therefore the arguments of each *Step I*, *Step II* etc extends to resonant points as well. However the number of *new points* to be taken into account on each step is given by the right-hand expression of (3.14) and therefore R needs to be redefined

$$R := h^{1-d} + \varepsilon^{3/2}h^{-d-\sigma}. \tag{3.17}$$

This leads to the final expression (1.15) for υ. Theorem 1.3 is proven.

[14] Recall, that $\mathcal{A}^0$ is diagonal matrix.

4 Discussion

4.1 Improving υ

Can we improve (increase) expression for υ given by (1.15)? I do not know if one can do anything with the restriction $\upsilon \le \epsilon\varepsilon^{-\frac{3}{2}(d-1)}h^{d(d-1)}$ which is due to resonant points, but restriction $\upsilon \le \epsilon h^{(d-1)^2}$ could be improved for $d \ge 3$, which makes sense only if

$$h \le h \le h^{\frac{2}{3}-\sigma}. \tag{4.1}$$

Indeed, on Step n, $n \ge 2$, we need to take into account only non-resonant points belonging to the set

$$\mathcal{J} := h(\Gamma^* + \xi) \cap \{\xi\colon |\mathcal{A}^0(\xi) - \tau| \le C\upsilon_{n-1}h\}. \tag{4.2}$$

Determination of upper estimate for such number falls into realm of the Number Theory. I am familiar only with the estimate

$$\#\mathcal{J} \le Ch^{1-d}\upsilon_{n-1} + Ch^{2-d-2/(d+1)}, \tag{4.3}$$

which follows from Theorem at page 224 of [Gui]. Probably it was improved, but those improvement have no value here.

The second term in the right-hand expression of (4.2) is larger, however, the second term in the right-hand expression of (3.17) is still larger and therefore on each Step $n \ge 2$ we have $R := \varepsilon^{3/2}h^{-d-\sigma}$, and this leads us to the following improvement of Theorem 1.3:

Theorem 4.1. *In the framework of Theorem 1.1, under additional assumptions $d \ge 3$ and (4.1), the statement of Theorem 1.3 holds with*

$$\upsilon = \epsilon\varepsilon^{-3(d-2)/2}h^{d^2-d-1-\sigma} \tag{4.4}$$

with arbitrarily small exponent $\sigma > 0$. In particular, $\upsilon = \epsilon h^{d^2-5d/2+3-\sigma}$ for $\varepsilon = h$.

Remark 4.2. One can try to improve further (4.4) for $\varepsilon \le h$. In this case resonant points become the main obstacle. In the definition of resonant points we need to take $\rho = h^{1/2-\delta}$; however only resonant points ξ with

$$\mathfrak{X}(\xi) \cap \{\xi'\colon |\mathcal{A}^0(\xi') - \tau| \le C(\upsilon_{n-1}h + \varepsilon)\} \ne \emptyset$$

should be taken into account on n-th step.

4.2 Condition (1.14)

We know that for connected component Σ_τ this condition (1.14) is fulfilled automatically.

On the other hand, let $\Sigma_\tau = \bigcup_{1\le j\le p}\Sigma_\tau^{(j)}$ with connected $\Sigma_\tau^{(j)}$. Let $p=2$ and condition (1.14) be violated at each point of Σ_τ. Does it mean that $\Sigma_\tau^{(2)} = \Sigma_\tau^{(1)} + \eta$ (i.e. $\Sigma_\tau^{(1)}$ shifted by η)?

Next, let $\Sigma_\tau^{(j)} = \Sigma_\tau^{(1)} + \eta_j$ for $j = 2, \dots, q$. Then for these components instead of condition (1.14) one can impose the similar condition involving level surfaces $\sigma_{\tau,\varepsilon}$ of $\mathcal{A}^0(\xi) + \varepsilon B_0(\xi)$. This would affect only *Step I* of our analysis, leading to $\upsilon_{1,\mathsf{new}} := \min(\varepsilon h, \upsilon_1)$ with υ_1 defined without taking into account of antipodal points. Since $\upsilon_1 \le h^{d-1}$ anyway, under assumption $\varepsilon \ge h$ we get the same formulae for υ for $d\ge 3$ as stated in Theorems 1.3 and 4.1, while for $d=2$ we get

$$\upsilon = h\min(\varepsilon,\ \varepsilon^{-3/2}h^{\sigma}). \tag{4.5}$$

4.3 Differentiability

Definitely our result would follow from the asymptotics of the *density of states*

$$\mathsf{N}'_h(\tau) := \frac{d\mathsf{N}_h(\tau)}{d\tau} = (\kappa'_0(\tau) + o(1))h^{-d} \qquad \text{as}\quad h\to +0, \tag{4.6}$$

where

$$\mathsf{N}_h(\tau) = \int_{\mathcal{O}^*} \mathsf{N}_h(\xi,\tau)\,d\xi \tag{4.7}$$

is an *integrated density of states:*

$$\mathsf{N}_h(\xi,\tau) = \#\{\mu<\tau,\ \mu\ \text{ is an eigenvalue of }\ A_h(\xi)\}. \tag{4.8}$$

However, despite $\mathsf{N}_h(\xi,\tau)$ has a complete asymptotics (see f.e. [Ivr3]), we do not know anything about asymptotics of $\mathsf{N}'_h(\tau)$ (even $\mathsf{N}'_h(\tau)\asymp h^{-d}$ is unknown).

4.4 Bethe-Sommerfeld Conjecture for Almost Periodic Perturbations

While both the proof of Bethe-Sommerfeld conjecture and the statement of Theorem 1.3 rely upon periodicity, the conjecture itself (as stated in

Theorem 1.1) does not. It is only natural to try to prove it for almost periodic perturbations as in [Ivr3].

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100 years of Weyl's Law

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Abstract

We discuss the asymptotics of the eigenvalue counting function for partial differential operators and related expressions paying the most attention to the sharp asymptotics. We consider Weyl asymptotics, asymptotics with Weyl principal parts and correction terms and asymptotics with non-Weyl principal parts. Semiclassical microlocal analysis, propagation of singularities and related dynamics play crucial role.

We start from the general theory, then consider Schrödinger and Dirac operators with the strong magnetic field and, finally, applications to the asymptotics of the ground state energy of heavy atoms and molecules with or without a magnetic field.

1 Introduction

A Bit of History

In 1911, Hermann Weyl, who at that time was a young German mathematician specializing in partial differential and integral equations, proved the following remarkable asymptotic formula describing distribution of (large) eigenvalues of the Dirichlet Laplacian in a bounded domain $X \subset \mathbb{R}^d$:

$$\mathsf{N}(\lambda) = (2\pi)^{-d}\omega_d \operatorname{vol}(X)\lambda^{d/2}(1 + o(1)) \qquad \text{as } \lambda \to +\infty, \tag{1.1}$$

where $\mathsf{N}(\lambda)$ is the number of eigenvalues of the (positive) Laplacian, which are less than λ [1], ω_d is a volume of the unit ball in $\mathbb{R}^d$, $\operatorname{vol}(X)$ is the

[1] $\mathsf{N}(\lambda)$ is called the *eigenvalue counting function*.

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volume of X. This formula was actually conjectured independently by Arnold Sommerfeld [Som] and Hendrik Lorentz [Lor] in 1910 who stated the *Weyl's Law* as a conjecture based on the book of Lord Rayleigh "The Theory of Sound" (1887) (for details, see [ANPS]).

H. Weyl published several papers [2–5, W1](1911–1915) devoted to the eigenvalue asymptotics for the Laplace operator (and also the elasticity operator) in a bounded domain with regular boundary. In [W4], he published what is now known as *Weyl's conjecture*

$$\mathsf{N}(\lambda) = (2\pi)^{-d}\omega_d \operatorname{vol}(X)\lambda^{d/2} \mp \frac{1}{4}(2\pi)^{1-d}\omega_{d-1}\operatorname{vol}'(\partial X)\lambda^{(d-1)/2} \qquad \text{as } \lambda\to+\infty \tag{1.2}$$

for Dirichlet and Neumann boundary conditions respectively where $\operatorname{vol}'(\partial X)$ is the $(d-1)$-dimensional volume of $\partial X \in \mathscr{C}^\infty$. Both these formulae appear in the toy-model of a rectangular box $X = \{0 < x_1 < a_1, \dots, 0 < x_d < a_d\}$ and then $\mathsf{N}(\lambda)$ is the number of integer lattice points in the part of ellipsoid $\{z_1^2/a_1^2 + \dots + z_d^2/a_d^2 < \pi^2\lambda\}$ with $z_j > 0$ and $z_j \ge 0$ for Dirichlet and Neumann boundary conditions respectively[2)].

After his pioneering work, a huge number of papers devoted to spectral asymptotics were published. Among the authors were numerous prominent mathematicians.

After H. Weyl, the next big step was made by Richard Courant [Cour](1920), who further developed the variational method and recovered the remainder estimate $O(\lambda^{(d-1)/2}\log\lambda)$. The variational method was developed further by many mathematicians, but it lead to generalizations rather than to getting sharp remainder estimates and we postpone its discussion until Section 3. Here we mention only Mikhail Birman, Elliott Lieb and Barry Simon and their schools.

The next development was due to Torsten Carleman [C1, C2](1934, 1936) who invented the *Tauberian method* and was probably the first to consider an arbitrary spacial dimension (H. Weyl and R. Courant considered only dimensions 2 and 3) followed by Boris Levitan [Lev1](1952) and V. G. Avakumovič [Av](1956) who, applied *hyperbolic operator method* (see Section 1) to recover the remainder estimate $O(\lambda^{(d-1)/2})$, but only for closed manifolds and also for $e(x, x, \lambda)$ away from the boundary[3)].

[2)] Finding sharp asymptotics of the number of the lattice points in the inflated domain is an important problem of the number theory.

[3)] Where here and below $e(x, y, \lambda)$ is the Schwartz kernel of the spectral projector.

After this, Lars Hörmander [Hör1, Hör2](1968, 1969) applied Fourier integral operators in the framework of this method. Hans Duistermaat and Victor Guillemin [DG](1975) recovered the remainder estimate $o(\lambda^{(d-1)/2})$ under the assumption that

(1.3) The set of all periodic geodesics has measure 0

observing that for the sphere neither this assumption nor (1.2) hold. Here, we consider the phase space T^*X equipped with the standard measure $dxd\xi$ where X is a manifold[4]. This was a very important step since it connected the sharp spectral asymptotics with classical dynamics.

The main obstacle was the impossibility to construct the parametrix of the hyperbolic problem near the boundary[5]. This obstacle was partially circumvented by Robert Seeley [See1, See2](1978, 1980) who recovered remainder estimate $O(\lambda^{(d-1)/2})$; his approach we will consider in Subsection 4. Finally the Author [Ivr1](1980), using very different approach, proved (1.2) under assumption that

(1.4) The set of all periodic geodesic billiards has measure 0,

which obviously generalizes (1.3). Using this approach, the Author in [Ivr2] (1982) proved (1.1) and (1.2) for elliptic systems on manifolds without boundary; (1.2) was proven under certain assumption similar to (1.3).

The new approaches were further developed during the 35 years to follow and many new ideas were implemented. The purpose of this article is to provide a brief and rather incomplete survey of the results and techniques. Beforehand, let us mention that the field was drastically transformed.

First, at that time, in addition to the problem that we described above, there were similar but distinct problems which we describe by examples:

(b) Find the asymptotics as $\lambda \to +\infty$ of $\mathsf{N}(\lambda)$ for the Schrödinger operator $\Delta + V(x)$ in $\mathbb{R}^d$ with potential $V(x) \to +\infty$ at infinity;

(c) Find the asymptotics as $\lambda \to -0$ of $\mathsf{N}(\lambda)$ for the Schrödinger operator in $\mathbb{R}^d$ with potential $V(x) \to -0$ at infinity (decaying more slowly than $|x|^{-2}$);

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[4] In fact the general scalar pseudodifferential operator and Hamiltonian trajectories of its principal symbol were considered.

[5] Or even inside for elliptic systems with the eigenvalues of the principal symbol having the variable multiplicity.

(d) Find the asymptotics as $h \to +0$ of $\mathsf{N}^-(h)$ the number of the negative eigenvalues for the Schrödinger operator $h^2\Delta + V(x)$.

These four problems were being studied separately albeit by rather similar methods. However, it turned out that the latter problem (d) is more fundamental than the others which could be reduced to it by the variational *Birman-Schwinger principle*.

Second, we should study the *local semiclassical spectral asymptotics*, i.e. the asymptotics of $\int e(x,x,0)\psi(x)\,dx$ where $\psi \in \mathscr{C}_0^\infty$ supported in the ball of radius 1 in which[6] V is of magnitude 1 [7]. By means of scaling we generalize these results for ψ supported in the ball of radius γ in which[6] V is of magnitude ρ with $\rho\gamma \ge h$ because in scaling $h \mapsto h/\rho\gamma$. Then in the general case we apply partition of unity with *scaling functions* $\gamma(x)$ and $\rho(x)$.

Third, in the *singular zone* $\{x:\ \rho(x)\gamma(x) \le h\}$b we can apply variational estimates and combine them with the semiclassical estimates in the *regular zone* $\{x:\ \rho(x)\gamma(x) \ge h\}$. It allows us to consider domains and operators with singularities.

Some further developments will be either discussed or mentioned in the next sections. Currently, I am working on the Monster book [Ivr4] which summarizes this development. It is almost ready and is available online and we will often refer to it for details, exact statements and proofs.

Finally, I should mention that in addition to the variational methods and method of hyperbolic operator, other methods were developed: other Tauberian methods (like the method of the heat equation or the method of resolvent) and the almost-spectral projector method [ST]. However, we will neither use nor even discuss them; for survey of different methods, see [RSS].

Method of the Hyperbolic Operator

The method of the hyperbolic operator is one of the Tauberian methods proposed by T. Carleman. Applied to the Laplace operator, it was designed as follows: let $e(x,y,\lambda)$ be the Schwartz kernel of a spectral projector and

[6] Actually, in the proportionally larger ball.

[7] Sometimes, however, we consider *pointwise semiclassical spectral asymptotics*, i.e. asymptotics of $e(x,x,0)$.

let

$$u(x,y,t)=\int_0^\infty \cos(\lambda t)\,d_\lambda e(x,y,\lambda^2); \tag{1.5}$$

observe, that now λ^2 is the spectral parameter. Then, $u(x,y,t)$ is a *propagator* of the corresponding wave equation and satisfies

$$u_{tt}+\Delta u=0, \tag{1.6}$$

$$u|_{t=0}=\delta(x-y),\quad u|_{t=0}=0 \tag{1.7}$$

(recall that Δ is a positive Laplacian).

Now we need to construct the solution of (1.6)–(1.7) and recover $e(x,y,t)$ from (1.5). However, excluding some special cases, we can construct the solution $u(x,y,t)$ only modulo smooth functions and only for $t:|t|\le T$, where usually T is a small constant. It leads to

$$F_{t\to\tau}\bigl(\bar\chi_T(t)u(x,x,t)\bigr)=T\int\hat{\bar\chi}((\lambda-\tau)T)\,d_\lambda e(x,x,\lambda^2)= \\ c_0(x)\lambda^{d-1}+c_1(x)\lambda^{d-2}+O(\lambda^{d-3}) \tag{1.8}$$

where F denotes the Fourier transform, $\bar\chi\in\mathscr{C}_0^\infty(-1,1)$, $\bar\chi(0)=1$, $\bar\chi'(0)=0$ and $\bar\chi_T(t)=\bar\chi(t/T)$ [8].

Then using Hörmander's Tauberian theorem[9], we can recover

$$e(x,x,\lambda^2)=c_0(x)d^{-1}\lambda^d+O(\lambda^{d-1}T^{-1}). \tag{1.9}$$

To get the remainder estimate $o(\lambda^{d-1})$ instead, we need some extra arguments. First, the asymptotics (1.8) holds with a cut-off:

$$F_{t\to\tau}\bigl(\bar\chi_T(t)(Q_xu)(x,x,t)\bigr)=T\int\hat{\bar\chi}((\lambda-\tau)T)\,d_\lambda (Q_xe)(x,x,\lambda^2)= \\ c_{0Q}(x)\lambda^{d-1}+c_{1Q}(x)\lambda^{d-2}+O_T(\lambda^{d-3}) \tag{1.10}$$

where $Q_x=Q(x,D_x)$ is a 0-order pseudo-differewntial operator (acting with respect to x only, before we set $x=y$; and $T=T_0$ is a small enough constant. Then the Tauberian theory implies that

$$(Q_xe)(x,x,\lambda^2)=c_{0Q}(x)d^{-1}\lambda^d+c_{1Q}(x)(d-1)^{-1}\lambda^{d-1}+ \\ O\bigl(\lambda^{d-1}T^{-1}\upmu(\operatorname{supp}(Q))\bigr)+o_{Q,T}\bigl(\lambda^{d-1}\bigr) \tag{1.11}$$

[8] In fact, there is a complete decomposition.

[9] Which was already known to Boris Levitan.

where $\mu = \frac{dxd\xi}{dg}$ is a natural measure on the *energy level surface* $\Sigma = \{(x,\xi) : g(x,\xi) = 1\}$ and we denote by $\mathsf{supp}(Q)$ the support of the symbol $Q(x,\xi)$.

On the other hand, propagation of singularities (which we discuss in more details later) implies that if for any point $(x,\xi) \in \mathsf{supp}(Q)$ geodesics starting there are not periodic with periods $\le T$ then asymptotics (1.10) and (1.11) hold with T.

Now, under the assumption (1.4), for any $T \ge T_0$ and $\varepsilon > 0$, we can select Q_1 and Q_2, such that $Q_1 + Q_2 = I$, $\mu(\mathsf{supp}(Q_1)) \le \varepsilon$ and for $(x,\xi) \in \mathsf{supp}(Q_2)$ geodesics starting from it are not periodic with periods $\le T$. Then, combining (1.11) with Q_1, T_0 and with Q_2, T, we arrive to

$$e(x,x,\lambda^2) = c_0(x)d^{-1}\lambda^d + c_1(x)(d-1)^{-1}\lambda^{d-1} + O\bigl(\lambda^{d-1}(T^{-1}+\varepsilon)\bigr) + o_{\varepsilon,T}(\lambda^{d-1}) \tag{1.12}$$

with arbitrarily large T and arbitrarily small $\varepsilon > 0$ and therefore

$$e(x,x,\lambda^2) = c_0(x)d^{-1}\lambda^d + c_1(d-1)^{-1}\lambda^{d-1} + O(\lambda^{d-1}T^{-1}). \tag{1.13}$$

holds. In these settings, $c_1 = 0$.

More delicate analysis of the propagation of singularities allows under certain very restrictive assumptions to the geodesic flow to boost the remainder estimate to $O(\lambda^{d-1}/\log\lambda)$ and even to $O(\lambda^{d-1-\delta})$ with a sufficiently small exponent $\delta > 0$.

2 Local Semiclassical Spectral Asymptotics

Asymptotics Inside the Domain

As we mentioned, the approach described above was based on the representation of the solution $u(x,y,t)$ by an oscillatory integral and does not fare well in (i) domains with boundaries because of the trajectories tangent to the boundary and (ii) for matrix operators whose principal symbols have eigenvalues of variable multiplicity. Let us describe our main method. We start by discussing matrix operators on closed manifolds.

So, let us consider a self-adjoint elliptic matrix operator $A(x,D)$ of order m. For simplicity, let us assume that this operator is semibounded from below and we are interested in $N(\lambda)$, the number of eigenvalues not exceeding λ, as $\lambda \to +\infty$. In other words, we are looking for the number $\mathsf{N}^-(h)$ of negative eigenvalues of the operator $\lambda^{-1}A(x,D) - I = H(x,hD,h)$ with $h = \lambda^{-1/m}$ [10].

Propagation of Singularities

Thus, we are now dealing with the semiclassical asymptotics. Therefore, instead of individual functions, we should consider families of functions depending on the *semiclassical parameter* h [11] and we need a *semiclassical microlocal analysis*. We call such family *temperate* if $\|u_h\| \le Ch^{-M}$ where $\|\cdot\|$ denotes usual $\mathscr{L}^2$-norm.

We say that $u := u_h$ is s*-negligible* at $(\bar{x},\bar{\xi}) \in T^*\mathbb{R}^d$ if there exists a symbol $\phi(x,\xi)$, $\phi(\bar{x},\bar{\xi}) = 1$ such that $\|\phi(x,hD)u_h\| = O(h^s)$. We call the *wave front set of* u_h the set of points at which u_h is not negligible and denote by $\mathsf{WF}^s(u_h)$; this is a closed set. Here, $-\infty < s \le \infty$.

Our first result is rather trivial: if $P = P(x,hD,h)$,

$$WF^s(u) \subset WF^s(Pu) \cup \mathsf{Char}(P) \tag{2.1}$$

where $\mathsf{Char}(P) = \{(x,\xi), \det P^0(x,\xi) = 0\}$; we call $P^0(x,\xi) := P(x,\xi,0)$ the *principal symbol* of P and $\mathsf{Char}(P)$ the *characteristic set* of L.

We need to study the propagation of singularities (wave front sets). To do this, we need the following definition:

Definition 2.1. Let P^0 be a Hermitian matrix. Then P is *microhyperbolic at* (x,ξ) *in the direction* $\ell \in T(T^*\mathbb{R}^d)$, $|\ell| \asymp 1$ if

$$\langle (\ell P^0)(x,\xi)v, v\rangle \ge \epsilon |v|^2 - C|P^0(x,\xi)v|^2 \qquad \forall v \tag{2.2}$$

with constants $\epsilon, C > 0$ [12].

Then we have the following statement which can be proven by the *method of the positive commutator*:

Theorem 2.2. *Let $P = P(x,hD,h)$ be an h-pseudodifferential operator with a Hermitian principal symbol. Let $\Omega \Subset T^*\mathbb{R}^d$ and let $\phi_j \in \mathscr{C}^\infty$ be real-valued functions such that P is microhyperbolic in Ω in the directions $\nabla^\# \phi_j$,*

---

[10] If operator is not semi-bounded we consider the number of eigenvalues in the interval $(0,\lambda)$ (or $(-\lambda,0)$) which could be reduced to the asymptotics of the number of eigenvalues in the interval $(-1,0)$ (or $(0,1)$) of $H(x,hD,h)$.

[11] Which in quantum mechanics is called Planck constant and usually is denoted by $\hbar$.

[12] Here and below ℓP^0 in is the action of the vector field ℓ upon P^0.

$j = 1, \dots, J$ where $\nabla^{\#}\phi = \langle(\nabla_\xi\phi), \nabla_x\rangle - \langle(\nabla_x\phi), \nabla_\xi\rangle$ is the Hamiltonian field generated by ϕ.

Let u be tempered and suppose that

$$\mathsf{WF}^{s+1}(Pu) \cap \Omega \cap \{\phi_1 \le 0\} \cap \dots \cap \{\phi_J \le 0\} = \emptyset, \tag{2.3}$$

$$\mathsf{WF}^{s}(u) \cap \partial\Omega \cap \{\phi_1 \le 0\} \cap \dots \cap \{\phi_J \le 0\} = \emptyset. \tag{2.4}$$

Then,

$$\mathsf{WF}^{s}(u) \cap \Omega \cap \{\phi_1 \le 0\} \cap \dots \cap \{\phi_J \le 0\} = \emptyset. \tag{2.5}$$

Proof. This is Theorem 2.1.2 from [Ivr4]. See the proof and discussion there. □

The above theorem immediately implies:

Corollary 2.3. *Let $H = H(x, hD, h)$ be an h-pseudodifferential operator with a Hermitian principal symbol and let $P = hD_t - H$. Let us assume that*

$$|\partial_{x,\xi} H^0 v| \le C_0|v| + C|(H^0 - \bar\tau)v| \qquad \forall v. \tag{2.6}$$

Let $u(x, y, t)$ be the Schwartz kernel of $e^{ih^{-1}tH}$.

(i) For a small constant $T^* > 0$,

$$WF(u) \cap \{|t| \le T^*,\ \tau = \bar\tau\} \subset \{|x - y|^2 + |\xi + \eta|^2 \le (C_0 t)^2\}. \tag{2.7}$$

(ii) Assume that H is microhyperbolic in some direction $\ell = \ell(x, \xi)$ at the point (x, ξ) at the energy level $\bar\tau$ [13]. Then for a small constant $T^* > 0$,

$$WF(u) \cap \{0 \le \pm t \le T^*,\ \tau = \bar\tau\} \subset \{\pm(\langle\ell_x, x - y\rangle + \langle\ell_\xi, \xi + \eta\rangle) \ge \pm\epsilon_0 t\}. \tag{2.8}$$

Proof. It is sufficient to prove the above statements for $t \ge 0$. We apply Theorem 2.2 with

(i) $\phi_1 = t$ and $\phi_2 = t - C_0^{-1}(|x - \bar x|^2 + \epsilon^2)^{\frac12} + \varepsilon$,

(ii) $\phi_1 = t$ and $\phi_2 = (\langle\ell_x, x - y\rangle + \langle\ell_\xi, \xi + \eta\rangle) - \epsilon_0 t + \varepsilon$,

[13] Which means that $H - \bar\tau$ is microhyperbolic in the sense of Definition 2.1.

where $\varepsilon > 0$ is arbitrarily small. □

Corollary 2.4. *(i) In the framework of Corollary 2.3(ii) with* $\ell = (\ell_x, 0)$, *the inequality*

$$|F_{t\to h^{-1}\tau}\chi_T(t)(Q_{1x} u\, {}^tQ_{2y})(x,x,t)| \le C_s h^{-d}(h/|t|)^s \tag{2.9}$$

holds for all s, $\tau : |\tau - \bar\tau| \le \epsilon$, $h \le |t| \lesssim T \le T^*$ *where* $Q_{1x} = Q_1(x, hD_x)$, $Q_{2y} = Q_2(y, hD_y)$ *are operators with compact supports,* ${}^tQ_2$ *is the dual rather than the adjoint operator and we write it to the right of the function,* $\chi \in \mathscr{C}_0^\infty([-1,-\frac{1}{2}] \cup [\frac{1}{2}, 1])$, $\chi_T(t) = \chi(t/T)$, *and* ϵ, T^* *are small positive constants.*

(ii) In particular, we get the estimate $O(h^s)$ *as* $T_* := h^{1-\delta} \le |t| \le T \le T^*$.

(iii) More generally, when $\ell = (\ell_x, \ell_\xi)$, *the same estimates hold for the distribution* $\sigma_{Q_1,Q_2}(t) = \int (Q_{1x} u\, {}^tQ_{2y})(x,x,t)\, dx$.

Proof. (i) If $t \asymp 1$, (2.9) immediately follows from Corollary 2.3(ii). Consider $t \asymp T$ with $h \le T \le T^*$ and make the rescaling $t \mapsto t/T$, $x \mapsto (x-y)/T$, $h \mapsto h/T$. We arrive to the same estimate (with $T^{-d}(h/T)^s$ in the right-hand expression where the factor T^{-d} is due to the fact that $u(x,y,t)$ is a density with respect to y). The transition from $|t| \asymp T$ to $|t| \lesssim T$ is trivial.

(ii) Statement (ii) follows immediately from Statement (i).

(iii) Statement (iii) follows immediately from Statements (i) and (ii) if we apply the metaplectic transformation $(x,\xi) \mapsto (x - B\xi, \xi)$ with a symmetric real matrix B. □

Therefore under the corresponding microhyperbolicity condition, we can construct $(Q_{1x} u\, {}^tQ_{2y})(x,x,t)$ or $\sigma_{Q_1,Q_2}(t)$ for $|t| \le T_*$ and then we automatically get it for $|t| \le T^*$. Since the time interval $|t| \le T_*$ is very short, we are able to apply the successive approximation method.

Successive Approximation Method

Let us consider the propagator $u(x,y,t)$. Recall that it satisfies the equations

$$(hD_t - H)u = 0, \tag{2.10}$$

$$u|_{t=0} = \delta(x-y)I \tag{2.11}$$

and therefore,

$$(hD_t - H)u^{\pm}\,{}^tQ_{2y} = \mp ih\delta(t)\delta(x-y)\,{}^tQ_{2y}, \tag{2.12}$$

where $u^{\pm} = u\theta(\pm t)$, θ is the Heaviside function, I is the unit matrix, $Q_{1x} = Q_1(x, hD_x)$, $Q_{2y} = Q_2(y, hD_y)$ have compact supports, ${}^tQ$ is the *dual operator*[14)] and we write operators with respect to y on the right from u in accordance with the notations of matrix theory.

Then,

$$(hD_t - \bar{H})u^{\pm}\,{}^tQ_{2y} = H'u \mp ih\delta(t)\delta(x-y)\,{}^tQ_{2y}I \tag{2.13}$$

with $\bar{H} = H(y, hD_x, 0)$ obtained from H by freezing $x = y$ and skipping lower order terms and $H' = H'(x, y, hD_x, h) = H - \bar{H}$. Therefore,

$$u^{\pm}\,{}^tQ_{2y} = \bar{G}^{\pm}ihH'u^{\pm}\,{}^tQ_{2y} \pm ih\bar{G}^{\mp}\delta(t)\delta(x-y)\,{}^tQ_{2y}I. \tag{2.14}$$

Iterating, we conclude that

$$u^{\pm}\,{}^tQ_{2y} = \sum_{0\le n\le N-1} (\bar{G}^{\pm}ihH')^n\bar{u}^{\pm}\,{}^tQ_{2y} + (\bar{G}^{\pm}ihH')^N u^{\pm}\,{}^tQ_{2y}, \tag{2.15}$$

$$\bar{u}^{\pm} = \mp ih\bar{G}^{\pm}\delta(t)\delta(x-y)\,{}^tQ_{2y}I \tag{2.16}$$

where $\bar{G}^{\pm}$ is a parametrix of the problem

$$(ihD_t - \bar{H})v = f, \qquad \operatorname{supp}(v) \subset \{\pm t \ge 0\} \tag{2.17}$$

and $G^{\pm}$ is a parametrix of the same problem problem albeit for H.

Observe that

$$H' = \sum_{1\le|\alpha|+m\le N-1} (x-y)^{\alpha}h^m R_{\alpha,m}(y, hD_x) + \sum_{|\alpha|+m=N} (x-y)^{\alpha}h^m R_{\alpha,m}(x, y, hD_x); \tag{2.18}$$

therefore due to the finite speed of propagation, its norm does not exceed CT as long as we only consider strips $\Pi^{\pm}_T := \{0 \le \pm t \le T\}$. Meanwhile, due to the Duhamel's integral, the operator norms of $G^{\pm}$ and $\bar{G}^{\pm}$ from $\mathscr{L}^2(\Pi^{\pm}_T)$ to $\mathscr{L}^2(\Pi^{\pm}_T)$ do not exceed $Ch^{-1}T$ and therefore each next term in the successive

14) I.e. ${}^tQv = (Q^*v^{\dagger})^{\dagger}$ where $v^{\dagger}$ is the complex conjugate to v.

approximations (2.15) acquires an extra factor $Ch^{-1}T^2 = O(h^\delta)$ as long as $T \le h^{\frac{1}{2}(1+\delta)}$ and the remainder term is $O(h^s)$ if N is large enough.

To calculate the terms of the successive approximations, let us apply h-Fourier transform $F_{(x,t)\to h^{-1}(\xi,\tau)}$ with $\xi \in \mathbb{R}^d$, $\tau \in \mathbb{C}_\mp := \{\tau : \mp \operatorname{Im}\tau > 0\}$ and observe that $\delta(t)\delta(x-y) \mapsto (2\pi)^{-d-1}e^{-ih^{-1}\langle y,\eta\rangle}$, ${}^tQ_{2y}$ and $R_{\alpha,m}$ become multiplication by $Q_2(y,\eta)$ and $R_{\alpha,m}(y,\xi)$ respectively, and $\bar{G}^\pm$ becomes multiplication by $(\tau - H^0(y,\xi))^{-1}$. Meanwhile, $(x_j - y_j)$ becomes $-ih\partial_{\xi_j}$.

Therefore the right-hand expression of (2.15) without the remainder term becomes a sum of terms $\mp i\mathcal{F}_m(y,\xi,\tau)h^{m+1}e^{-ih^{-1}\langle y,\eta\rangle}$ with $m \ge 0$ and $\mathcal{F}_m(y,\xi,\tau)$ the sum of terms of the type

$$(\tau - H^0(y,\xi))^{-1}b_*(y,\xi)(\tau - H^0(y,\xi))^{-1}b_*(y,\xi)\cdots b_*(y,\xi)\times (\tau - H^0(y,\xi))^{-1}Q_2(y,\eta) \tag{2.19}$$

with no more than $2m+1$ factors $(\tau - H^0(y,\xi))^{-1}$. Here, the b_* are regular symbols. In particular,

$$\mathcal{F}_0(y,\xi,\tau) = (2\pi)^{-d-1}(\tau - H^0(y,\xi))^{-1}Q_2(y,\eta). \tag{2.20}$$

If we add the expressions for u^+ and u^- instead of $\mathcal{F}_m(y,\xi,\tau)$ with $\tau \in \mathbb{C}_\mp$, we get the distributions $\bigl(\mathcal{F}_m(y,\xi,\tau+i0) - \mathcal{F}_m(y,\xi,\tau-i0)\bigr)$ with $\tau \in \mathbb{R}$.

Applying the inverse h-Fourier transform with respect to x, operator Q_{1x}, and setting $x = y$, we cancel the factor $e^{-ih^{-1}\langle y,\eta\rangle}$ and gain a factor of h^{-d}. Thus we arrive to the Proposition 2.5(i) below; applying Corollary 2.4(ii) and (iii), we arrive to its Statements (ii) and (iii). We also need to use

$$u(x,y,t) = \int e^{ih^{-1}t\tau}\, d_\tau e(x,y,\tau). \tag{2.21}$$

Proposition 2.5. *(i) As* $T_* = h^{1-\delta} \le T \le h^{\frac{1}{2}+\delta}$ *and* $\bar\chi \in \mathscr{C}_0^\infty([-1,1])$

$$T\int \widehat{\bar\chi}\bigl((\lambda-\tau)Th^{-1}\bigr)\, d_\tau(Q_{1x}e\,{}^tQ_{2y})(y,y,\tau) \sim \sum_{m\ge 0} h^{-d+m}T\int \widehat{\bar\chi}\bigl((\lambda-\tau)Th^{-1}\bigr)\kappa'_m(y,\tau)d\tau, \tag{2.22}$$

where $\widehat{\bar\chi}$ *is the Fourier transform of* $\bar\chi$ *and*

$$\kappa'_m(y) = \int \bigl(\mathcal{F}_m(y,\xi,\tau+i0) - \mathcal{F}_m(y,\xi,\tau-i0)\bigr)\, d\eta. \tag{2.23}$$

(ii) If H is microhyperbolic on the energy level $\bar\tau$ on $\mathsf{supp}(Q_2)$ in some direction ℓ with $\ell_x = 0$ then (2.21) *holds with $T_* \le T \le T^*$, $|\lambda - \bar\tau| \le \epsilon$, where T^* is a small constant.*

(iii) On the other hand, if $\ell_x \ne 0$, then (2.21) *still holds with $T \le T^*$, albeit only after integration with respect to y:*

$$T\int \widehat{\bar\chi}\bigl((\lambda-\tau)Th^{-1}\bigr)\,d_\tau\Bigl(\int (Q_{1x}e\,{}^tQ_{2y})(y,y,\tau)\,dy\Bigr) \sim \sum_{m\ge 0} h^{-d+m}T\int \widehat{\bar\chi}\bigl((\lambda-\tau)Th^{-1}\bigr)\varkappa'_m(\tau)\,d\tau \tag{2.24}$$

with

$$\varkappa'_m(\tau) = \iint \bigl(\mathcal{F}_m(y,\xi,\tau+i0) - \mathcal{F}_m(y,\xi,\tau-i0)\bigr)\,dyd\eta. \tag{2.25}$$

For details, proofs and generalizations, see Section 4.3 of [Ivr4].

Recovering Spectral Asymptotics

Let $\alpha(\tau)$ denote $(Q_{1x}e\,{}^tQ_{2y})(y,y,\tau)$ (which may be integrated with respect to y) and $\beta(\tau)$ denote the convolution of its derivative $\alpha'(\tau)$ with $T\widehat{\bar\chi}(\tau T/h)$. To recover $\alpha(\tau)$ from $\beta(\tau)$, we apply *Tauberian methods*. First of all, we observe that under the corresponding microhyperbolicity condition the distribution $\kappa'_m(y,\tau)$ or $\varkappa'_m(\tau)$ is smooth and the right-hand side expression of (2.22) or (2.24) does not exceed Ch^{-d+1}.

Let us take $Q_1 = Q_2$; then $\alpha(y,\tau)$ or $\alpha(\tau)$ is a monotone non-decreasing matrix function of τ. We choose a Hörmander function[15] $\bar\chi(t)$ and estimate the left-hand expressions of (2.22) or (2.24) from below by

$$\epsilon_0 T\bigl(\alpha(\lambda+hT^{-1}) - \alpha(\lambda-hT^{-1})\bigr),$$

which implies that $\bigl(\alpha(\lambda+hT^{-1})-\alpha(\lambda-hT^{-1})\bigr) \le CT^{-1}h^{-d+1}$ and therefore

$$|\alpha(\lambda)-\alpha(\mu)| \le Ch^{-d+1}|\lambda-\mu| + CT^{-1}h^{-d+1} \tag{2.26}$$

as $\lambda,\mu \in (\bar\tau-\epsilon,\bar\tau+\epsilon)$. Then (2.26) automatically holds, even if Q_1 and Q_2 are not necessarily equal.

---

[15] I.e. a compactly supported function with positive Fourier transform.

Further, (2.26) implies that

$$|\alpha(\lambda)-\alpha(\mu)-h^{-1}\int_\mu^\lambda \beta(\tau)\,d\tau|\le CT^{-1}h^{-d+1} \tag{2.27}$$

and therefore

$$|\int\Bigl(\alpha(\lambda)-\alpha(\mu)-h^{-1}\int_\mu^\lambda \beta(\tau)\,d\tau\Bigr)\phi(\mu)\,d\mu|\le CT^{-1}h^{-d+1} \tag{2.28}$$

if $\bar\chi=1$ on $[-\frac{1}{2},\frac{1}{2}]$, $\lambda,\mu\in(\bar\tau-\epsilon,\bar\tau+\epsilon)$ and $\phi\in\mathscr{C}_0^\infty((\bar\tau-\epsilon,\bar\tau+\epsilon))$ with $\int\phi(\tau)\,d\tau=1$.

On the other hand, even without the microhyperbolicity condition, our successive approximation construction is not entirely useless. Let us apply $\varphi_L(hD_t-\lambda)$ with $\varphi\in\mathscr{C}_0^\infty([-1,1])$ and $L\ge h^{\frac{1}{2}-\delta}$, and then set $t=0$. We arrive to

$$\int\varphi((\tau-\lambda)L^{-1})\bigl(\alpha'(\tau)-\beta(\tau)\bigr)\,d\tau=O(h^\infty). \tag{2.29}$$

This allows us to extend (2.28) to $\phi\in\mathscr{C}_0^\infty(bR))$ with $\int\phi(\tau)\,d\tau=1$. For full details and generalizations, see Section 4.4 of [Ivr4].

Thus, we have proved:

Theorem 2.6. *Let $H=H(x,hD,h)$ be a self-adjoint operator. Then,*

(i) The following asymptotics holds for $L\ge h^{\frac{1}{2}-\delta}$:

$$\int\phi((\tau-\lambda)L^{-1})\Bigl(d_\tau(Q_{1x}e\,{}^tQ_{2y})(y,y,\tau)-\sum_{m\ge 0}h^{-d+m}\kappa'(y,\tau)\,d\tau\Bigr) = O(h^\infty). \tag{2.30}$$

(ii) Let H be microhyperbolic on the energy level $\bar\tau$ in some direction ℓ with $\ell_x=0$. Then for $|\lambda-\bar\tau|\le\epsilon$,

$$(Q_{1x}e\,{}^tQ_{2y})(y,y,\lambda)=h^{-d}\kappa_0(y,\lambda)+O(h^{-d+1}) \tag{2.31}$$

with $\kappa_m(y,\lambda):=\int_{-\infty}^\lambda\kappa'_m(y,\tau)\,d\tau$.

(iii) Let H be microhyperbolic on the energy level $\bar\tau$ in some direction ℓ. Then for $|\lambda-\bar\tau|\le\epsilon$,

$$\int (Q_{1x} e\, {}^tQ_{2y})(y,y,\lambda)\,dy = h^{-d}\varkappa_0(\lambda) + O(h^{-d+1}) \tag{2.32}$$

with $\varkappa_m(y) := \int_{-\infty}^{\lambda} \varkappa'_m(\tau)\,d\tau$.

(iv) In particular, it follows from (2.20) *that*

$$\kappa_0(\lambda,x) = (2\pi)^{-d}\int q_1^0(x,\xi)\theta(\lambda - H^0(x,\xi))q_2^0(x,\xi)\,d\xi \tag{2.33}$$

and

$$\varkappa_0(\lambda) = (2\pi)^{-d}\int q_1^0(x,\xi)\theta(\lambda - H^0(x,\xi))q_2^0(x,\xi)\,dxd\xi \tag{2.34}$$

Remark 2.7. (i) So far we have assumed that Q_1, Q_2 had compactly supported symbols in (x,ξ). Assuming that these symbols are compactly supported with respect to x only, in particular when $Q_1=\psi(x)$, $Q_2=1$, with $\psi\in\mathscr{C}_0^\infty(X)$, we need to assume that

$$\{\xi : \exists x\in X : \operatorname{Spec} H^0(x,\xi)\cap(-\infty,\lambda+\epsilon_0]\ne\emptyset\} \text{ is a compact set.} \tag{2.35}$$

(ii) If we assume only that

$$\{\xi : \exists x\in X : \operatorname{Spec} H^0(x,\xi)\cap(\mu-\epsilon_0,\lambda+\epsilon_0]\ne\emptyset\} \text{ is a compact set,} \tag{2.36}$$

instead of (2.31) and (2.32), we get

$$|(Q_{1x} e\, {}^tQ_{2y})(y,y,\lambda,\mu) - h^{-1}\kappa_0(y,\lambda,\mu)| \le Ch^{-d+1} \tag{2.37}$$

and

$$|\iint (Q_{1x} e\, {}^tQ_{2y})(y,y,\lambda,\mu)\,dy - h^{-1}\varkappa_0(\lambda,\mu)| \le Ch^{-d+1}, \tag{2.38}$$

where $\mu\le\lambda$, $e(x,y,\lambda,\mu) := e(x,y,\lambda) - e(x,y,\mu)$, $\kappa_m(y,\lambda) := \int_\mu^\lambda \kappa'_m(y,\tau)\,d\tau$, $\varkappa_m(y,\lambda) := \int_\mu^\lambda \varkappa'_m(y,\tau)\,d\tau$ and we assume that the corresponding microhyperbolicity assumption is fulfilled on both energy levels μ and λ.

(iii) If $H^0(x,\xi)$ is an elliptic symbol which is positively homogeneous of degree $m > 0$ with respect to ξ, then the microhyperbolicity condition is fulfilled with $\ell = (0, \pm\xi)$ on energy levels $\tau \neq 0$. Furthermore, the compactness condition of (ii) is fulfilled, and if $H^0(x,\xi)$ is also positive-definite, then the compactness condition of (i) is also fulfilled.

Second Term and Dynamics

Propagation of Singularities To derive two-term asymptotics, one can use the scheme described in Section 1, albeit one needs to describe the propagation of singularities. For matrix operators, this may be slightly tricky.

Let us introduce the *characteristic symbol* $g(\mathsf{x},\upxi) := \det(\tau - H^0(\mathsf{x},\xi))$ where $\mathsf{x} = (x_0, x)$, $\upxi = (\xi_0,\xi)$ etc; then $\mathsf{Char}(\xi_0 - H(x,\xi)) = \{(x,\upxi) : g(x,\upxi) = 0\}$. Let ξ_0 be a root of multiplicity r of $g(x,\xi_0,\xi)$; then $g^{(\alpha)}_{(\beta)}(x,\upxi) = 0$ for all $\alpha,\beta : |\alpha| + |\beta| < r$. Let us consider the r-jet of g at such a point:

$$g_{(x,\upxi)}(y,\upeta) := \sum_{\alpha,\beta:|\alpha|+|\beta|<r} \frac{1}{\alpha!\beta!} g^{(\alpha)}_{(\beta)}(x,\upxi) y^\beta \upeta^\alpha; \tag{2.39}$$

it is a hyperbolic polynomial with respect to η_0. Consider its *hyperbolicity cone* $K(x,\upxi)$, which is the connected component of $\{(\mathsf{y};\upeta) \in \mathbb{R}^{2d+2} : g_{(x,\upxi)}(\mathsf{y},\upeta) \neq 0\}$ containing $\{(y,\eta) : \eta_0 = 1, y = \eta = 0\}$ and the *dual hyperbolicity cone*

$$K^\#(x,\upxi) = \{(\mathsf{y}',\upeta') : \langle \mathsf{y}',\upeta\rangle - \langle \mathsf{y},\upeta'\rangle > 0\} \subset \{y_0 = 0\}. \tag{2.40}$$

Definition 2.8. (i) An absolutely continuous curve $(\mathsf{x}(t),\upxi(t))$ (with $x_0 = t$) is called a *generalized Hamiltonian trajectory* if a.e.

$$(1, \frac{dx}{dt}; \frac{d\upxi}{dt}) \in K^\#(x,\xi_0,\xi). \tag{2.41}$$

Note that $\xi_0 = \tau$ remains constant along the trajectory.

(ii) Let $\mathcal{K}^\pm(x,\upxi)$ denote the union of all generalized Hamiltonian trajectories issued from $(x,\upxi)$ in the direction of increasing/decreasing t.

If $g = \alpha g_1^r$ where $\alpha \ne 0$ and $g_1 = 0 \implies \nabla g_1 \ne 0$, the generalized Hamiltonian trajectories are just (ordinary) Hamiltonian trajectories of g_1 and $\mathcal{K}^\pm(x,\xi)$ are just half-trajectories[16)].

The following theorem follows from Theorem 2.2:

Theorem 2.9. *If $u(x,y,t)$ is the Schwartz kernel of $e^{ih^{-1}tH}$, then*

$$\mathsf{WF}(u) \subset \{(x,\xi;y,-\eta;t,\tau) : \pm t > 0, (t,x;\tau,\xi) \in K^\pm(0,y;\tau,\eta)\}. \tag{2.42}$$

Then, we obtain:

Corollary 2.10. *In the framework of Theorem 2.9,*

$$\mathsf{WF}(\sigma_{Q_1,Q_2}(t)) \subset \{(t,\tau) :\ \exists (x,\xi) :\ (t,x;\tau,\xi) \in \mathcal{K}^\pm(0,x;\tau,\xi)\}, \tag{2.43}$$

and for any x,

$$\mathsf{WF}(Q_{1x} u\, {}^tQ_{2y}) \subset \{(t,\tau) :\ \exists \xi,\eta :\ (t,x;\tau,\xi) \in \mathcal{K}^\pm(0,x;\tau,\eta)\}. \tag{2.44}$$

Definition 2.11. (i) A *periodic point* is a point (x,ξ) which satisfies $(t,x;\tau,\xi) \in \mathcal{K}^\pm(0,x;\tau,\xi)$ for some $t \ne 0$.

(ii) A *loop point* is a point x which satisfies $(t,x;\tau,\xi) \in \mathcal{K}^\pm(0,x;\tau,\eta)$ for some $t \ne 0$, ξ,η; we call η a *loop direction.*

Application to Spectral Asymptotics Combining Corollary 2.10 with the arguments of Section 1, we arrive to

Theorem 2.12. *(i) In the framework of Theorem 2.6(ii) let for some x the set of all loop directions at point x on energy level λ have measure 0*[17)]*. Then,*

$$(Q_{1x} e\, {}^tQ_{2y})(y,y,\lambda) = h^{-d}\kappa_0(y,\lambda) + h^{1-d}\kappa_1(y,\lambda) + o(h^{-d+1}). \tag{2.45}$$

(ii) In the framework of Theorem 2.6(iii), suppose that the set of all periodic points on energy level λ has measure 0[18)]*. Then,*

$$\int (Q_{1x} e\, {}^tQ_{2y})(y,y,\lambda)\, dy = h^{-d}\varkappa_0(\lambda) + h^{1-d}\varkappa_1(\lambda) + o(h^{-d+1}). \tag{2.46}$$

[16)] Since $e^{ih^{-1}tH}$ describes evolution with revert time, time is also reverted along (generalized) Hamiltonian trajectories.

[17)] There exists a natural measure $\mu_{\lambda,x}$ on $\{\xi : \det(\lambda - H^0(x,\xi)) = 0\}$.

[18)] There exists a natural measure μ_λ on $\{(x,\xi) : \det(\lambda - H^0(x,\xi)) = 0\}$.

Remark 2.13. (i) When studying propagation, we can allow H to also depend on $x_0 = t$; for all details and proofs, see Sections 2.1 and 2.2 of [Ivr4].

(ii) Recall that $e(x,y,\lambda)$ is the Schwartz kernel of $\theta(\lambda - H)$. We can also consider $e_\nu(x,y,\tau)$ which is the Schwartz kernel of $(\lambda - H)_+^\nu := (\lambda - H)^\nu\theta(\lambda - H)$ with $\nu \geq 0$. Then in the Tauberian arguments, $h^{-d}\times(h/T)$ is replaced by $h^{-d}\times(h/T)^{1+\nu}$ and then in the framework of Theorem 2.6(ii) and (iii) remainder estimates are $O(h^{-d+1+\nu})$ and in the framework of Theorem 2.6(i) and (ii), the remainder estimates are $o(h^{-d+1+\nu})$; sure, in the asymptotics one should include all the necessary terms $\kappa_m h^{-d+m}$ or $\varkappa_m h^{-d+m}$ [19].

(iii) Under more restrictive conditions on Hamiltonian trajectories instead of T an arbitrarily large constant, we can take T depending on h [20]; see Section 2.4 of [Ivr4]. Usually, we can take $T = \epsilon|\log h|$ or even $T = h^{-\delta}$.

Then in the remainder estimate, the main term is

$$C\bigl(\mu(\Pi_{T,\gamma})h^{-d+1} + h^{-d+1+\nu}T^{-1-\nu}\bigr),$$

where $\Pi_{T,\gamma}$ is the set of all points $z = (x,\xi)$ (on the given energy level) such that $\mathsf{dist}(\Psi_t(z),z) \leq \gamma$ for some $t \in (\epsilon, T)$ and $\gamma = h^{1/2-\delta'}$. Here, however, we assume that either H^0 is scalar or its eigenvalues have constant multiplicities and apply the Heisenberg approach to the long-term evolution.

Then the remainder estimates could be improved to $O(h^{-d+1+\nu}|\log h|^{-1-\nu})$ or even to $O(h^{-d+1+\nu+\delta})$ respectively. As examples, we can consider the geodesic flow on a Riemannian manifold with negative sectional curvature (log case) and the completely integrable non-periodic Hamiltonian flow (power case). For all details and proofs, see Section 4.5 of [Ivr4].

Rescaling Technique

The results we proved are very uniform: as long as we know that operator in question is self-adjoint and that the smoothness and non-degeneracy conditions are fulfilled uniformly in $B(\bar{x},1)$, then all asymptotics are also uniform (as $x \in B(\bar{x},\frac{1}{2})$ or $\mathsf{supp}(\psi) \subset B(\bar{x},\frac{1}{2})$). Then these results could self-improve.

[19] Here, we need to assume that H is semi-bounded from below; otherwise some modifications are required.

[20] Usually these restrictions are $T \leq h^{-\delta}$ and $|D\Psi_t(z)| \leq h^{-\delta}$ with sufficiently small $\delta > 0$.

Here we consider only the Schrödinger operator away from the boundary; but the approach could be generalized for a wider class of operators. For generalizations, details and proofs, see Chapter 5 of [Ivr4].

Proposition 2.14. *Consider the Schrödinger operator. Assume that* $\rho\gamma \ge h$ *and in* $B(\bar{x},\gamma)\subset X$*,*

$$|\partial^\alpha g^{jk}| \le c_\alpha \gamma^{-|\alpha|}, \qquad |\partial^\alpha V| \le c_\alpha \rho^2 \gamma^{-|\alpha|}. \tag{2.47$_{1,2}$}$$

Then,

(i) In $B(\bar{x},\frac{1}{2}\gamma)$*,*

$$e(x,x,0) \le C\rho^d h^{-d}. \tag{2.48}$$

(ii) If in addition $|V| + |\nabla V|\gamma \ge \epsilon\rho^2$*, then for* $\operatorname{supp}(\psi)\subset B(\bar{x},\frac{1}{2}\gamma)$ *such that* $|\partial^\alpha\psi| \le c_\alpha\gamma^{-|\alpha|}$*,*

$$\Bigl|\int \bigl(e(x,x,0) - \kappa_0 V_-^{d/2}\bigr)\,dx\Bigr| \le C\rho^{d-1}\gamma^{d-1}h^{1-d}; \tag{2.49}$$

(iii) If in addition $|V| \ge \epsilon\rho^2$ *in* $B(\bar{x},\gamma)$ *then*

$$|e(x,x,0) - \kappa_0 V_-^{d/2}| \le C\rho^{d-1}\gamma^{-1}h^{1-d}; \tag{2.50}$$

(iv) If in addition $V \ge \epsilon\rho^2$ *in* $B(\bar{x},\gamma)$*, then for any* s*,*

$$|e(x,x,0)| \le C\rho^{d-s}\gamma^{-s}h^{s-d}. \tag{2.51}$$

Proof. Indeed, we have already proved this in the special case $\rho=\gamma=1$, $h\le 1$. In the general case, we can reduce the problem to the special case by rescaling $x\mapsto x\gamma^{-1}$, $\tau\mapsto\tau\rho^{-2}$ (so we multiply operator by ρ^{-2}) and then automatically $h\mapsto\hbar = h\rho^{-1}\gamma^{-1}$. Recall that $e(x,y,\tau)$ is a function with respect to x but a density with respect to y so an extra factor γ^{-d} appears in the right-hand expressions. □

Let us assume that the conditions $(2.47)_{1,2}$ are fulfilled with $\rho=\gamma=1$. We want to get rid of the non-degeneracy assumption $|V|\asymp 1$ in the pointwise asymptotics. Let us introduce the *scaling function* $\gamma(x)$ and also $\rho(x)$

$$\gamma(x) = \epsilon|V(x)| + \bar{\gamma} \quad \text{with} \quad \bar{\gamma} = h^{\frac{2}{3}}, \qquad \rho(x) = \gamma(x)^{\frac{1}{2}}. \tag{2.52}$$

One can easily see that

$$|\nabla\gamma| \le \frac{1}{2}, \qquad \rho\gamma \ge h, \tag{2.53}$$

$(2.47)_{1,2}$ are fulfilled and either $|V| \ge \epsilon\rho^2$ or $\rho\gamma \asymp h$ and therefore (2.50) holds ($\hbar \asymp 1$ as $\rho\gamma \asymp h$ and no non-degeneracy condition is needed). Note that for $d \ge 3$, the right-hand expression of (2.50) is $O(h^{1-d})$ and for $d = 1, 2$, it is $O(h^{-\frac{2}{3}d})$. So, we got rid of the non-degeneracy assumption $|V| \asymp 1$, and the remainder estimate deteriorated only for $d = 1, 2$.

Remark 2.15. (i) We can improve the estimates for $d = 1, 2$ to $O(h^{\frac{1}{3}-\frac{2}{3}d})$, but then we will need to add some correction terms first under the assumption $|V| + |\nabla V| \asymp 1$ and then get rid of it by rescaling; these correction terms are of boundary-layer type (near $V = 0$) and are $O(h^{-\frac{2}{3}d})$ and are due to short loops. For details, see Theorems 5.3.11 and 5.3.16 of [Ivr4].

(ii) If $d = 2$, then under the assumption $|V| + |\nabla V| \asymp 1$, the weight $\rho^{-1}\gamma^{-1}$ is integrable, and we arrive to the local asymptotics with the remainder estimate $O(h^{1-d})$.

(iii) We want to get rid of the non-degeneracy assumption $|V| + |\nabla V| \asymp 1$ in the local asymptotics. We can do it with the scaling function

$$\gamma(x) = \epsilon\bigl(|V(x)| + |\nabla V|^2\bigr)^{\frac{1}{2}} + \bar{\gamma} \quad \text{with } \ \bar{\gamma} = h^{\frac{1}{2}}, \qquad \rho(x) = \gamma(x). \tag{2.54}$$

Then for $d = 2$, we recover remainder the estimate $O(h^{-1})$; while for $d = 1$, the remainder estimate $O(h^{-\frac{1}{2}})$ which could be improved further up to $O(1)$ under some extremely weak non-degeneracy assumption or to $O(h^{-\delta})$ with an arbitrarily small exponent $\delta > 0$ without it.

(iv) If $d \ge 2$, then in the framework of Theorem 2.12(i), we can get rid of the non-degeneracy assumption as well. This is true for the magnetic Schrödinger operator as well if $d \ge 2$; when $d = 2$, some modification of the statement is required; see Remark 5.3.4 of [Ivr4].

(v) Furthermore, if we consider asymptotics for $\operatorname{Tr}((\lambda - H)_+^{\nu}\psi)$ (see Remark 2.13(ii)) with $\nu > 0$ then in the local asymptotics, we get the remainder estimate $O(h^{1-d+s})$ without any non-degeneracy assumptions. For details, see Theorem 5.3.5 of [Ivr4].

Operators with Periodic Trajectories

Preliminary Analysis Consider a scalar operator H. For simplicity, assume that X is a compact closed manifold. Assume that all the Hamiltonian trajectories are periodic (with periods not exceeding $C(\mu)$ on the energy levels $\lambda \le \mu$). Then the period depends only on the energy level and let $T(\lambda)$ be the minimal period such that all trajectories on the energy level λ are $T(\lambda)$ periodic[21)].

Without any loss of the generality, one can assume that $T(\lambda) = 1$. Indeed, we can replace H by $f(H)$ with $f'(\lambda) = 1/T(\lambda)$. Then,

$$e^{\nabla^\# H^0} = I \tag{2.55}$$

and therefore,

$$e^{ih^{-1}H} = e^{i\varepsilon h^{-1}B}, \tag{2.56}$$

where $B = B(x, hD, h)$ is an h-pseudo-differential operator which could be selected to commute with H, at this point, $\varepsilon = h$. Then, $H_0 = H - \varepsilon B$ satisfies

$$e^{ih^{-1}H_0} = I \implies \mathsf{Spec}(H_0) \subset 2\pi h\mathbb{Z}; \tag{2.57}$$

we call this *quantum periodicity* in contrast to the *classical periodicity* (2.55).

We can calculate the multiplicity $\mathsf{N}_{k,h} = O(h^{1-d})$ of the eigenvalue $2\pi hk$ with $k \in \mathbb{Z}$ modulo $O(h^\infty)$. The formula is rather complicated especially since subperiodic trajectories[21)] cause the redistribution of multiplicities between eigenvalues (however, this causes no more than $O(h^{1-d+r})$ error).

We consider $H := H_\varepsilon = H_0 + \varepsilon B$ as a perturbation of H_0 and we assume only that $\varepsilon \ll 1$. If $\varepsilon \le \epsilon_0 h$, the spectrum of H consists of *eigenvalue clusters* of the width $C_0\varepsilon$ separated by *spectral gaps* of the width $\asymp h$, but if $\varepsilon \ge \epsilon_0 h$, these clusters may overlap.

Long Range Evolution Consider

$$e^{ih^{-1}tH} = e^{ih^{-1}tH_0}e^{-ih^{-1}t\varepsilon B} = e^{ih^{-1}t'H_0}e^{ih^{-1}t''B} \tag{2.58}$$

[21)] However, there could be *subperiodic trajectories*, i.e. trajectories periodic with period $T(\lambda)/p$ with $p = 2, 3, \ldots$. It is known that the set Λ_p of subperiodic trajectories with subperiod $T(\lambda)/p$ is a union of symplectic submanifolds $\Lambda_{p,r}$ of codimension $2r$.

with $t''=\varepsilon t$, $t'=t-\lfloor t\rfloor$. We now have a *fast evolution* $e^{ih^{-1}t'H_0}$ and a *slow evolution* $e^{ih^{-1}t''B}$ and both t', t'' are bounded as $|t|\le T^*:=\varepsilon^{-1}$. Therefore, we can trace the evolution up to time T^*.

Let the following non-degeneracy assumption be fulfilled:

$$|\nabla_{\Sigma(\lambda)} b|\ge \epsilon_0, \tag{2.59}$$

where b is the principal symbol of B, $\Sigma(\lambda):=\{(x,\xi):\ H^0(x,\xi)=\lambda\}$ and $\nabla_{\Sigma(\lambda)}$ is the gradient along $\Sigma(\lambda)$. Then using our methods, we can prove that

$$|F_{t\to h^{-1}\tau}\chi_T(t)\int u(x,x,t)\psi(x)\,dx|\le CTh^{1-d}(h/\varepsilon T)^s, \tag{2.60}$$

and therefore

$$F_{t\to h^{-1}\tau}\bar\chi_T(t)\int u(x,x,t)\psi(x)\,dx|\le Ch^{1-d}(\varepsilon^{-1}h+1) \tag{2.61}$$

for $\epsilon_0(\varepsilon^{-1}h+1)\le T\le \epsilon_0\varepsilon^{-1}$; recall that $\chi\in\mathscr{C}_0^\infty([-1,-\frac{1}{2}]\cup[\frac{1}{2},1]$ and $\bar\chi\in\mathscr{C}_0^\infty([-1,1]$, $\bar\chi=1$ on $[-\frac{1}{2},\frac{1}{2}]$.

Then the Tauberian error does not exceed the right-hand expression of (2.61) multiplied by $T^{*\,-1}\asymp\varepsilon$, i.e. $Ch^{1-d}(\varepsilon+h)$. In the Tauberian expression, we need to take $T=\epsilon_0(\varepsilon^{-1}h^{1-\delta}+1)$.

Calculations We can pass from Tauberian expression to a more explicit one. Observe that the contribution to the former are produced only by time intervals $t\in[n-h^{1-\delta},n+h^{1-\delta}]$ with $|n|\le T_*$; contribution of the remaining interval will be either negligible (if there are no subperiodic trajectories) or $O(h^{2-d})$ (if such trajectories exist). Such an interval with $n=0$ produces the standard Weyl expression.

Consider $n\ne 0$. Then the contribution of such intervals lead to a correction term

$$\mathsf{N}_{\mathsf{corr},Q_1,Q_2}(\lambda):=(2\pi)^{-d}h^{1-d}\int_{\Sigma_\tau} q_1^0\Upsilon_1\bigl(h^{-1}(H^0-\varepsilon b)\bigr)\,d\upmu_\tau q_2^0, \tag{2.62}$$

where $\Upsilon_1(t)=2\pi\lceil\frac{t}{2\pi}\rceil-t+\frac{1}{2}$.

Theorem 2.16. *Under assumptions* (2.55), (2.56), (2.59) *and* $\varepsilon\ge h^M$,

$$\begin{aligned}\int(Q_{1x}e\,{}^tQ_{2y})(y,y,\lambda)\,dy &= h^{-d}\varkappa_{0,Q_1,Q_2}(\lambda)\\ &+h^{1-d}\varkappa_{1,Q_1,Q_2}(\lambda)+\mathsf{N}_{\mathsf{corr},Q_1,Q_2}(\lambda)+O\bigl(h^{1-d}(\varepsilon+h)\bigr).\end{aligned} \tag{2.63}$$

For a more general statement with (2.59) replaced by a weaker non-degeneration assumption, see Theorem 6.2.24 of [Ivr4]. Further, we can skip a correction term (2.62) if $\varepsilon \ge h^{1-\delta}$; while if $h^M \le \varepsilon \le h^{1-\delta}$, this term is $O(h^{1-d}(h/\varepsilon)^s)$ for $\varepsilon \ge h$ and of magnitude h^{1-d} for $h^M \le \varepsilon \le h$.

For further generalizations, details and proofs, see Sections 6.2 and 6.3 of [Ivr4]. For related spectral asymptotics for a family of commuting operators, see Section 6.1 of [Ivr4].

One can also consider the case when there is a massive set of periodic trajectories, yet non-periodic trajectories exist. For details, see [SV1] and Subsection 6.3.7 of [Ivr4].

Boundary Value Problems

Preliminary Analysis

Let X be a domain in $\mathbb{R}^d$ with boundary ∂X and H an h-differential matrix operator which is self-adjoint in $\mathscr{L}^2(X)$ under the h-differential boundary conditions. Again, we are interested in the local and pointwise spectral asymptotics, i.e. those of $\int e(x,x,0)\psi(x)\,dx$ with $\psi \in \mathscr{C}_0^\infty(B(0,\frac{1}{2}))$ and of $e(x,x,0)$ with $x \in B(0,\frac{1}{2})$.

Assume that in $B(0,1)$, everything is good: ∂X and coefficients of H are smooth, H is ξ-microhyperbolic on the energy levels $\lambda_{1,2}$ ($\lambda_1 < \lambda_2$) and also H is elliptic as a differential operator, i.e.

$$\|H(x,\xi)v\| \ge (\epsilon_0|\xi|^m - C_0)\|v\| \qquad \forall v \quad \forall x \in B(0,1)\ \forall \xi. \tag{2.64}$$

Then,

$$e(x,x,\lambda_1,\lambda_2) = \kappa_0(x,\lambda_1,\lambda_2)h^{-d} + O(h^{1-d}\gamma(x)^{-1}) \tag{2.65}$$

for $x \in B(0,\frac{1}{2})$ and $\gamma(x) \ge h$,

$$\kappa_0(x,\lambda_1,\lambda_2) = (2\pi)^{-d}\int \big(\theta(\lambda_2 - H^0(x,\xi)) - \theta(\lambda_1 - H^0(x,\xi))\big)\,d\xi \tag{2.66}$$

and $\gamma(x) = \frac{1}{2}\mathsf{dist}(x,\partial X)$.

Indeed, the scaling $x \mapsto (x-y)/\gamma$ and $h \mapsto \hbar/\gamma$ brings us into the framework of Theorem 2.6(ii) because ξ-microhyperbolicity (in contrast to the (x,ξ)-microhyperbolicity) survives such rescaling. Then,

$$\int_{\{x:\,\gamma(x)\ge h\}} \bigl(e(x,x,\lambda_1,\lambda_2) - h^{-d}\kappa_0(x,\lambda_1,\lambda_2)\bigr)\psi(x)\,dx = O(h^{1-d}\log h), \tag{2.67}$$

since $\int_{\{x:\,\gamma(x)\ge h\}}\gamma(x)^{-1}\,dx \asymp |\log h|$.

One can easily show that if the boundary value problem for H is elliptic then

$$e(x,x,\lambda_1,\lambda_2) = O(h^{-d}) \tag{2.68}$$

and therefore,

$$\int \bigl(e(x,x,\lambda_1,\lambda_2) - h^{-d}\kappa_0(x,\lambda_1,\lambda_2)\bigr)\psi(x)\,dx = O(h^{1-d}\log h). \tag{2.69}$$

To improve this remainder estimate, one needs to improve (2.67) rather than (2.65) but to get sharper asymptotics, we need to improve both. We will implement the same scheme as inside the domain.

Propagation of Singularities

Toy-Model: Schrödinger Operator Let us consider the Schrödinger operator

$$H \coloneqq h^2\Delta + V(x) \tag{2.70}$$

with the boundary condition

$$\bigl(\alpha(x)h\partial_\nu + \beta(x)\bigr)v|_{\partial X} = 0, \tag{2.71}$$

where

$$\Delta = \sum_{j,k} D_j g^{jk} D_k, \qquad \partial_\nu = \sum_j g^{j1}\partial_j \tag{2.72}$$

is derivative in the direction of the inner normal ν (we assume that $X = \{x:\, x_1 > 0\}$ locally[22)]), α and β are real-valued and do not vanish simultaneously. Without any loss of the generality, we can assume that locally

$$g^{j1} = \delta_{j1}. \tag{2.73}$$

[22)] I.e. in intersection with $B(0,1)$.

First of all, near the boundary, we can study the propagation of singularities using the same scheme as in Subsection 2 as long as $\phi_j(x,\xi)=\phi_j(x,\xi')$ do not depend on the component of ξ which is "normal to the boundary". The intuitive way to explain why one needs this is that at reflections, ξ_1 changes by a jump.

For the Schrödinger operator, it is sufficient for our needs: near *glancing points* (x,ξ') (which are points such that $x_1=0$ and the set $\{\xi_1 : H^0(x',\xi',\xi_1)=\tau\}$ consists of exactly one point), we can apply this method. On the other hand, near other points, we can construct the solution by traditional methods of oscillatory integrals.

It is convenient to decompose $u(x,y,t)$ into the sum

$$u=u^0(x,y,t)+u^1(x,y,t), \tag{2.74}$$

where $u^0(x,y,t)$ is a *free space solution* (without boundary) which we studied in Subsection 2 and $u^1:=u-u^0$ is a *reflected wave*.

Observe that even for the Schrödinger operator, we cannot claim that the singularity of $u(x,x,t)$ at $t=0$ is isolated. The reason are *short loops* made by trajectories which reflect from the boundary in the normal direction and follow the same path in the opposite direction. However, these short loops affect neither $u(x,x,t)$ at the points of the boundary nor $u(x,x,t)$ integrated in any direction transversal to the boundary (and thus do not affect $\sigma_\psi(t)$ defined below).

Furthermore, they do not affect $(Q_{1x}u\,{}^tQ_{2y})(x,x,t)$ as long as at least one of operators $Q_j=Q_j(x,hD',hD_t)$ cuts them of. Then we get the estimate (2.9). Consider $Q_1=Q_2=1$. Then, if $V(x)-\lambda>0$, we get the same estimate at the point $x\in\partial X$. On the other hand, if either $V(x)-\lambda<0$ or $V(x)=\lambda,\ \nabla_{\partial X}V(x)\neq 0$ (where $\nabla_{\partial X}$ means "along ∂X") at each point of $\mathsf{supp}(\psi)$, we get the same estimate for $\sigma_\psi(x)=\int u(x,x,t)\,dx$. As usual, λ is an energy level.

Moreover, $\sigma^1_\psi(t)=\int u^1(x,x,t)\psi(x)\,dx$ satisfies

$$|F_{t\to h^{-1}\tau}\chi_T(t)\sigma^1_\psi(t)|\leq C_s h^{1-d}(h/|t|)^s. \tag{2.75}$$

In contrast to the Dirichlet ($\alpha=0$, $\beta=1$) or Neumann ($\alpha=1$, $\beta=0$) conditions, under the more general boundary condition (2.71), the classically forbidden level λ (i.e. with $\lambda<\inf_{B(0,1)}V$) may be not forbidden after all. Namely, in this zone, the operator hD_t-H is elliptic and we can construct the *Dirichlet-to-Neumann operator* $L : v|_{\partial X} \to h\partial_1 v|_{\partial X}$ as $(hD_t - H)v \equiv 0$. This is an h-pseudo-differential operator on ∂X with principal symbol

$$L^0(x', \xi', \tau) = -\bigl(V + \sum_{j,k\ge 2} g^{jk}\xi_j\xi_k - \tau\bigr)^{\frac{1}{2}}. \tag{2.76}$$

Then the boundary condition (2.71) becomes

$$Mw := (\alpha L + \beta)w \equiv 0, \qquad w = v|_{\partial X}. \tag{2.77}$$

The energy level $\lambda < V(x)$ is indeed forbidden if the operator M is elliptic as $\tau = \lambda$, i.e. if $M^0(x', \xi', \lambda) = \alpha L^0(x', \xi', \lambda) + \beta \ne 0$ for all ξ'; it happens as either $\alpha^{-1}\beta < 0$ or $W := V - \alpha^{-2}\beta^2 > \lambda$. Otherwise, to recover (2.75)[23], we assume that M is either ξ'-microhyperbolic or (x', ξ')-microhyperbolic ($W > \lambda$ and $W = \lambda \implies \nabla_{\partial X} W \ne 0$ respectively).

General Operators For more general operators and boundary value problems, we use similar arguments albeit not relying upon the representation of $u(x, y, t)$ via oscillatory integrals. It follows from (2.74) that

$$(hD_t - H)u^{1\,\pm} = 0, \tag{2.78}$$

$$Bu^{1\,\pm}|_{x_1=0} = -Bu^{0\,\pm}|_{x_1=0}, \tag{2.79}$$

where as before, $u^{k\,\pm} = u^k\theta(\pm t)$, $k = 0, 1$. Assuming that H satisfies (2.64), we reduce (2.78)–(2.79) to the problem

$$\mathcal{A}U^{1\,\pm} := (\mathcal{A}_0 hD_1 + \mathcal{A}_1)U^{1\,\pm} \equiv 0, \tag{2.80}$$

$$\mathcal{B}U^{1\,\pm}|_{x_1=0} = -\mathcal{B}U^{0\,\pm} \tag{2.81}$$

with $\mathcal{A}_k = \mathcal{A}_k(x, hD', hD_t)$, $\mathcal{B} = \mathcal{B}(x, hD', hD_t)$ and $U = S_x u\, {}^t S_y$ with $S = S(x, hD_x, hD_t)$ etc[24].

In a neighbourhood of any point $(\bar{x}', \bar{\xi}', \lambda)$, the operator $\mathcal{A}$ could be reduced to the block-diagonal form with blocks $\mathcal{A}_{kj}$ ($k = 0, 1$, $j = 1, \dots, N$) such that

(a) For each $j = 1, \dots, N-1$, the equation $\det(\mathcal{A}^0_{0j}\eta + \mathcal{A}^0_{1j}) = 0$ has a single real root η_j (at the point $(\bar{x}', \bar{\xi}', \lambda)$ only), η_j are distinct, and

[23] With d replaced by $d-1$.

[24] If H is a $\mathsf{D}\times\mathsf{D}$ matrix operator of order m then $\mathcal{A}$ and S are $m\mathsf{D}\times m\mathsf{D}$ and $m\mathsf{D}\times\mathsf{D}$ matrix operators, B and $\mathcal{B}$ are $\frac{1}{2}m\mathsf{D}\times\mathsf{D}$ and $\frac{1}{2}m\mathsf{D}\times m\mathsf{D}$ matrix operators respectively.

(b) $\mathcal{A}_{kN} = \begin{pmatrix} 0 & \mathcal{A}'_{kN} \\ \mathcal{A}''_{kN} & 0 \end{pmatrix}$ with $\det(\mathcal{A}'^{0}_{0N}\eta + \mathcal{A}'^{0}_{1N}) = 0$ and $\det(\mathcal{A}''^{0}_{0N}\eta + \mathcal{A}''^{0}_{1N}) = 0$ has only roots with $\operatorname{Im}\eta < 0$ and with $\operatorname{Im}\eta > 0$ respectively.

We can prove a statement similar to Theorem 2.2, but instead of functions $\phi_*(x,\xi)$, we now have arrays of functions $\phi_{*j}(x,t,\xi',\tau)$ ($j = 1,\dots,N-1$) coinciding with $\phi_{*N}(x',t,\xi',\tau)$ as $x_1 = 0$. Respectively, instead of microhyperbolicity of the operator in the direction $\ell \in T(T^*(X \times \mathbb{R}))$, we now have the *microhyperbolicty of the boundary value problem in the multidirection* $(\ell', \nu_1, \dots, \nu_{N-1}) \in T(T^*(\partial X \times \mathbb{R})) \times \mathbb{R}^{N-1}$; see Definition 3.1.4 of [Ivr4]. It includes the microhyperbolicity of $\mathcal{A}_j$ in the direction $(\ell', 0, \nu_j)$ for $j = 1,\dots,N-1$ and a condition invoking $\mathcal{A}_N$ and $\mathcal{B}$ and generalizing the microhyperbolicity of operator M for the Schrödinger operator. Respectively, instead of the microhyperbolicity of an operator in the direction $\nabla^{\#}\phi_*$, we want the microhyperbolicity in the multidirection $(\nabla'^{\#}\phi_*, \partial_1\phi_{*1}, \dots, \partial_1\phi_{*(N-1)})$.

As a corollary, under the microhyperbolicity assumption on the energy level λ, we prove estimates (2.9) for $\sigma^0_\psi(t)$, $\sigma_\psi(t)$ and (2.75) for $\sigma^1_\psi(t)$ as τ is close to λ. Furthermore, if the operator H is elliptic on this energy level then $\sigma^0_\psi(t)$ is negligible and (2.75) holds for $\sigma^1_\psi(t)$ and $\sigma_\psi(t)$.

For details, proofs and generalizations, see Chapter 3 of [Ivr4].

Successive Approximations Method

After the (2.9) and (2.75)-type estimates are established, we can apply the successive approximations method like in Subsection 2 but with some modifications: to construct $Bu^{0\pm}|_{x_1=0}$ and from it to construct $u^{1\pm}$, we freeze coefficients in $(y',0)$ rather than in y. As a result, we can calculate all terms in the asymptotics and under microhyperbolicity in the multidirection condition, we arrive to the formulae (2.24) for $e^0(.,.,\tau)$, $e^1(.,.,\tau)$ and $e(.,.,\tau)$ [25] with $m \geq 1$ for $e^1(.,.,\tau)$.

The formulae for $\varkappa^1_m(\tau)$ (and thus for $\varkappa_m(\tau) = \varkappa^0_m(\tau) + \varkappa^1_m(\tau)$ are however rather complicated and we do not write them here. For the Schrödinger operator with $V = 0$ and boundary condition (2.71), the calculation of $\varkappa^1_1(\tau)$ is done in [HA].

Similar formulae also hold if we take $x_1 = y_1 = 0$ and integrate over ∂X (but in this case $m \geq 0$ even for $e^1(.,.,\tau)$).

Furthermore, if $\ell'_x = 0$ and $\nu_1 = \dots = \nu_{N-1}$ in the condition of microhyperbolicity, we are able to get formulae for $e^0(x,x,\tau)$, $e^1(x,x,\tau)$ and

[25] With the obvious definitions of $e^0(.,.,\tau)$ and $e^1(.,.,\tau)$.

$e(x,x,\tau)$ without setting $x_1=0$ and without integrating but $e^1(x,x,\tau)$ is a boundary-layer type term.

For details and proofs, see Section 7.2 of [Ivr4].

Recovering Spectral Asymptotics

Repeating the arguments of Subsection 2, we can recover the local spectral asymptotics:

Theorem 2.17. *(i) Let an operator H be microhyperbolic on $\mathsf{supp}(\psi)$ on the energy levels λ_1 and λ_2 ($\lambda_1<\lambda_2$) and the boundary value (H,B) problem be microhyperbolic on $\mathsf{supp}(\psi)\cap\partial X$ on these energy levels. Then,*

$$\int_X e(y,y,\lambda_1,\lambda_2)\psi(y)\,dy = h^{-d}\int_X \kappa_0(y,\lambda_1,\lambda_2)\psi(y)\,dy + O(h^{-d+1}). \tag{2.82}$$

(ii) Suppose that an operator H is elliptic on $\mathsf{supp}(\psi)$ on the energy levels λ_1 and λ_2 ($\lambda_1<\lambda_2$)[26] *and the boundary value (H,B) problem is microhyperbolic on $\mathsf{supp}(\psi)\cap\partial X$ on these energy levels. Then,*

$$\int_X e(y,y,\lambda_1,\lambda_2)\psi(y)\,dy = h^{1-d}\int_X \kappa_1(y,\lambda_1,\lambda_2)\psi(y)\,dy + O(h^{-d+2}). \tag{2.83}$$

On the other hand, for the Schrödinger operator, we can calculate the contributions of near normal trajectories explicitly and then we arrive to:

Theorem 2.18. *Let (H,B) be the Schrödinger operator* (2.70)–(2.71) *and let $|V|\neq\lambda$ on $\mathsf{supp}(\psi)$. Then,*

$$e(y,y,\lambda) = h^{-d}\bigl(\kappa_0(x,\lambda)+\mathcal{Q}(x',\lambda;h^{-1}x_1)\bigr)+O(h^{-d+1}) \tag{2.84}$$

where $\mathcal{Q}$ depends on the "normal variables" (x',λ) and a "fast variable" $s=h^{-1}x_1$ and decays as $O(s^{-d+1/2})$ as $s\to+\infty$. Here, $x_1=\mathsf{dist}(x,\partial X)$.

For details, exact statement and proofs, see Section 8.1 of [Ivr4].

[26] Then, it is elliptic on all energy levels $\tau\in[\lambda_1,\lambda_2]$.

Second Term and Dynamics

As in Subsection 2, we can improve our asymptotics under certain conditions to the dynamics of propagation of singularities. However, in the case that the manifold has a non-empty boundary, propagation becomes really complicated. For Schrödinger operators, we can prove that singularities propagate along Hamiltonian billiards unless they "behave badly" that is become tangent to ∂X at some point or make an infinite number of reflections in finite time. However, the measure of *dead-end points*[27)] is 0.

Thus, applying the arguments of Section 1 we arrive to

Theorem 2.19. *Let $d \geq 2$, $|V-\lambda| + |\nabla V| \neq 0$ on $\mathsf{supp}(\psi)$ and $|V-\lambda| + |\nabla_{\partial X} V| \neq 0$ on $\mathsf{supp}(\psi) \cap \partial X$. Further, assume that the measure of periodic Hamiltonian billiards passing through points of $\{H^0(x,\xi)=0\} \cap \mathsf{supp}(\psi)$ is 0*[28)]*. Then,*

$$\int e(y,y,\lambda)\psi(y)\,dy = h^{-d}\int \kappa_0(y,\lambda)\psi(y)\,dy + o(h^{-d+1}). \tag{2.85}$$

Remark 2.20. If we are interested in the propagation of singularities without applications to spectral asymptotics, the answer is "singularities propagate along the generalized Hamiltonian billiards" (see Definition 3.2.2 in [Ivr4]).

One can easily show:

Theorem 2.21. *Let $d \geq 3$. Assume that we are in the framework of Theorem 2.17(ii). Further assume that the set of periodic trajectories of the Schrödinger operator on ∂X with potential W introduced after* (2.77) *has measure 0. Then,*

$$\int e(y,y,\lambda)\psi(y)\,dy = h^{1-d}\varkappa_{1,\psi}(\lambda) + h^{2-d}\varkappa_{2,\psi}(\lambda) + o(h^{-d+2}). \tag{2.86}$$

Remark 2.22. Analysis becomes much more complicated for more general operators even if we assume that the inner propagation is simple. For example, if the operator in question is essentially a collection of m Schrödinger operators intertwined through boundary conditions then every incidence ray after reflection generates up to m reflected rays and we have *branching*

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27) I.e. points $z \in \Sigma(\lambda)$ the billiard passing through which behaves badly.

28) There is a natural measure $dxd\xi : dH^0$.

Hamiltonian billiards. Here, a *dead-end point* is a point $z \in \Sigma(\lambda)$ such that *some of the branches* behave badly and a *periodic point* is a point $z \in \Sigma(\lambda)$ such that *some of the branches* return to it.

Assume that the sets of all periodic points and all dead-end points on the energy level $\Sigma(\lambda)$ have measure 0 (as shown in [SV2], the set of all dead-end points may have positive measure). Then, the two-term asymptotics could be recovered. However, the investigation of branching Hamiltonian billiards is a rather daunting task.

Rescaling Technique

The rescaling technique could be applied near ∂X as well. Assume that $\lambda = 0$. Then to get rid of the non-degeneracy assumption $V(x) \le -\epsilon$, we use scaling functions $\gamma(x)$ and $\rho(x)$ as in Subsection 2. It may happen that $B(x, \gamma(x)) \subset X$ or it may happen that $B(x, \gamma(x))$ intersects ∂X. In the former case, we are obviously done and in the latter case we are done as well because in the condition (2.71) we scale $\alpha \mapsto \alpha\rho\nu$, $\beta \mapsto \beta\nu$ where $\nu > 0$ is a parameter of our choice. Thus, in the pointwise asymptotics, we can get rid of this assumption for $d \ge 3$, and in the local asymptotics for $d \ge 2$ assuming that $|V| + |\nabla V| \asymp 1$ because the total measure of the balls of radii $\le \gamma$ which intersect ∂X is $O(\gamma)$. For details, exact statements and proofs, see Section 8.2 of [Ivr4].

Operators with Periodic Billiards

Simple Billiards Consider an operator on a manifold with boundary. Assume first that all the billiard trajectories (on energy levels close to λ) are *simple* (i.e. without branching) and periodic with a period bounded from above; then the period depends only on the energy level. Example: the Laplace-Beltrami operator on the semisphere. Under some non-degeneracy assumptions similar to (2.59), we can derive asymptotics similar to (2.63) but with two major differences:

(i) We assume that $\varepsilon \asymp h$ and recover remainder estimate only $O(h^{1-d+\delta})$; it is still good enough to have the second term of the non-standard type.

(ii) We can consider $b(x, \xi)$ (which is invariant with respect to the Hamiltonian billard flow) as a phase shift for one period. Now, however, it could be a result not only of the quantum drift as in Subsection 2, but also of an instant change of phase at the moment of the reflection.

For exact statements, details and proofs, see Subsection 8.3.2 of [Ivr4].

Branching Billiards with "Scattering" We now assume that the billiard branches but only one ("main") branch is typically periodic. For example, consider two Laplace-Beltrami operators intertwined through boundary conditions: one of them is an operator on the semisphere X_1 and another on the disk X_2 with ∂X_1 and ∂X_2 glued together. Then all billiards on X_1 are periodic but there exist nowhere dense sets $\Lambda_j(\lambda)$ of measure 0, such that the billiards passing through $\Sigma_j(\lambda) \setminus \Lambda_j(\lambda)$ and containing at least one segment in X_2 are not periodic. Assume also that the boundary conditions guarantee that at reflection, the "observable" part of energy escapes into X_2. Then to recover the sharp remainder estimates, we do not need a phase shift because for time $T \gg 1$, we have

$$T|F_{t\to h^{-1}\tau}\bar{\chi}_T(t)\, d_\tau e(y,y,\tau)\, dy| \le C_0 h^{1-d} \sum_{|n|\le T} q^n + o_T(h^{1-d}), \tag{2.87}$$

where $q \le 1$ estimates from above the "portion of energy" which goes back to X_1 at each reflection; if $q < 1$, as we have assumed the right-hand expression does not exceed $C_1 h^{1-d} + o_T(h^{1-d})$ and we recover asymptotics similar to (2.63) with the remainder estimate $o(h^{1-d})$.

For exact statements, details and proofs, see Subsection 8.3.3 of [Ivr4].

Two Periodic Billiards We can also consider the case when the billiards flows in X_1 and X_2 are both periodic but "magic" happens at reflections. For exact statements, details and proofs, see Subsection 8.3.4 of [Ivr4].

3 Global Asymptotics

In this section, we consider global spectral asymptotics. Here we are mainly interested in the asymptotics with respect to the spectral parameter λ. We consider mainly examples.

Weyl Asymptotics

Regular Theory

We start from examples in which we apply only the results of the previous Chapter 2 which may be combined with *Birman-Schwinger principle* and the rescaling technique.

Simple Results

Example 3.1. Consider a self-adjoint operator A with domain $\mathfrak{D}(A) = \{u : Bu|_{\partial X} = 0\}$. We assume that A is elliptic and the boundary value problem (A, B) is elliptic as well.

(i) We are interested in $\mathsf{N}(0, \lambda)$, the number of eigenvalues of A in $[0, \lambda)$. Instead we consider $\mathsf{N}(\lambda/2, \lambda)$, which is obviously equal to $\mathsf{N}_h(\frac{1}{2}, 1)$, the number of eigenvalues of $A_h = \lambda^{-1}A$ that lie in $[\frac{1}{2}, 1)$, with $h = \lambda^{-1/m}$ where m is the order of A. In fact, more is true: the principal symbols of semiclassical operators A_h and B_h coincide with the senior symbols of A and B. Then the microhyperbolicity conditions are satisfied and the semiclassical asymptotics with the remainder estimate $O(h^{1-d})$ hold which could be improved to two-term asymptotics under our standard non-periodicity condition. As a result, we obtain

$$\mathsf{N}(0, \lambda) = \varkappa_0 \lambda^{\frac{d}{m}} + O(\lambda^{\frac{d-1}{m}}) \tag{3.1}$$

and

$$\mathsf{N}(0, \lambda) = \varkappa_0 \lambda^{\frac{d}{m}} + \varkappa_1 \lambda^{\frac{d-1}{m}} + o(\lambda^{\frac{d-1}{m}}), \tag{3.2}$$

as $\lambda \to +\infty$ in the general case and under the standard non-periodicity condition respectively. Here,

$$\varkappa_0 = (2\pi)^{-d} \iint \boldsymbol{n}(x, \xi)\, dxd\xi \tag{3.3}$$

where $\boldsymbol{n}(x, \xi)$ is the number of eigenvalues of $A^0(x, \xi)$ in $(0, 1)$ and $m = m_A$ is the order of A.

(ii) Suppose that A_B is positive definite (then $m_A \geq 2$) and V is an operator of the order $m_B < m_A$, symmetric under the same boundary conditions. We are interested in $\mathsf{N}(0, \lambda)$, the number of eigenvalues of VA_B^{-1} in (λ^{-1}, ∞).

Using the Birman-Schwinger principle, we can again reduce the problem to the semiclassical one with $H = h^{m_A}A - h^{m_V}V$, $h = \lambda^{-1/m}$, $m = m_A - m_V$. The microhyperbolicity condition is fulfilled automatically unless $\xi = 0$ and $V^0(x,\xi)$ is degenerate. Still under certain appropriate assumptions about V^0, we can ensure microhyperbolicity (for $m_B = 0, 1$ only). Then (3.1) and (3.2) (the latter under standard non-periodicity condition) hold with $\boldsymbol{n}(x,\xi)$ the number of eigenvalues of $V^0(x,\xi)(A^0(x,\xi)^{-1})$ in $(1,\infty)$.

(iii) Alternatively, we can consider the case when V is positively defined (and A_B may be not).

(iv) For scalar operators, one can replace microhyperbolicity by a weaker non-degeneracy assumption. Furthermore, without any non-degeneracy assumption we arrive to one-term asymptotics with the remainder estimate $O(\lambda^{(d-1+\delta)/m})$.

(v) Also one can consider operators whose all Hamiltonian trajectories are periodic; in this case the oscillatory correction term appears.

(vi) Suppose the operator A_B has negative definite principal symbol but A_B is not semi-bounded from above and V is positive definite. Then instead of (3.1) or (3.2), we arrive to

$$\mathsf{N}(0,\lambda) = \varkappa_1\lambda^{\frac{d-1}{m}} + O(\lambda^{\frac{d-2}{m}}) \tag{3.4}$$

and

$$\mathsf{N}(0,\lambda) = \varkappa_1\lambda^{\frac{d-1}{m}} + \varkappa_2\lambda^{\frac{d-2}{m}} + o(\lambda^{\frac{d-2}{m}}), \tag{3.5}$$

(the latter under an appropriate non-periodicity assumption).

Fractional Laplacians The fractional Laplacian $\Lambda_{m,X}$ appears in the theory of stochastic processes. For $m > 0$, it is defined first on $\mathbb{R}^d$ as $\Delta^{m/2}$, and in a domain $X \subset \mathbb{R}^d$, it is defined as $\Lambda_{m,X}u = R_X\Delta^{m/2}(\theta_X u)$ where R_X is the restriction to X and θ_X is the characteristic function of X. It differs from the $m/2$-th power of the Dirichlet Laplacian in X and for $m \notin 2\mathbb{Z}$, it does not belong to the Boutet de Monvel's algebra. In particular, even if X is a bounded domain with $\partial X \in \mathscr{C}^\infty$ and $u \in \mathscr{C}^\infty(\bar{X})$, $\Lambda_{m,X}u$ does not necessarily belong to $\mathscr{C}^\infty(\bar{X})$ (smoothness is violated in the direction normal to ∂X).

Then the standard Weyl asymptotics (3.1) and (3.2) hold (the latter under standard non-periodicity condition) with the standard coefficient $\varkappa_0 = (2\pi)^{-d}\omega_{d-1}\,\mathsf{vol}_d(X)$ and with

$$\varkappa_{1,m} = (2\pi)^{1-d}\omega_{d-1}\sigma_m\,\mathsf{vol}_{d-1}(\partial X), \tag{3.6}$$

$$\sigma_m = \\ = \frac{d-1}{m}\iint_1^\infty \tau^{-(d-1)/m-1}\Bigl(e_m(x_1,x_1,\tau) - \pi^{-1}(\tau-1)^{1/m}\Bigr)\,dx_1 d\tau \tag{3.7}$$

where $e_m(x_1,y_1,\tau)$ is the Schwartz kernel of the spectral projector of operator

$$a_m = ((D_x^2+1)^{m/2})_{\mathsf{D}} \tag{3.8}$$

on $\mathbb{R}^+$. To prove this, we need to redo some analysis of Chapter 2. While tangent rays are treated exactly as for the ordinary Laplacian, normal rays require some extra work. However, we can show that the singularities coming along transversal rays do not stall at the boundary but reflect according the standard law. For exact statements, details and proofs, see [Ivr5].

Semiclassical Dirichlet-to-Neumann Operator Consider the Laplacian Δ in X. Assuming that λ is not an eigenvalue of Δ_{D}, we can introduce the Dirichlet-to-Neumann operator $L_\lambda : v \mapsto \lambda^{-\frac{1}{2}}\partial_\nu u|_{\partial X}$ where u is defined as $(\Delta-\lambda)u = 0$, $u|_{\partial X} = v$ and ν is the inner unit normal. Here, L_λ is a self-adjoint operator and we are interested in $\mathsf{N}_\lambda(a_1,a_2)$, the number of its eigenvalues in the interval $[a_1,a_2)$. Due to the Birman-Schwinger principle, it is equal to $N_h^-(a_1) - N_h^-(a_2)$ where $N_h^-(a)$ is the number of the negative eigenvalues of $h^2\Delta - 1$ under the boundary condition $(h\partial_\nu - a)u|_{\partial X} = 0$ and then we arrive to

$$\mathsf{N}_\lambda(a_1,a_2) = O(\lambda^{\frac{d-1}{m}}) \tag{3.9}$$

and

$$\mathsf{N}_\lambda(a_1,a_2) = \varkappa_1(a_1,a_2)\lambda^{\frac{d-1}{2}} + o(\lambda^{\frac{d-1}{2}}) \tag{3.10}$$

(the latter under a standard non-periodicity condition). For exact statements, details and proofs, see [HA].

Rescaling Technique We are interested in the asymptotics of either

$$\mathsf{N}^{-}(\lambda) = \int e(x,x,\lambda)\,dx \tag{3.11}$$

or

$$\mathsf{N}(\lambda_1,\lambda_2) = \int e(x,x,\lambda_1,\lambda_2)\,dx \qquad \text{with} \quad \lambda_1 < \lambda_2 : \tag{3.12}$$

with respect to either the spectral parameter(s), or semiclassical parameter(s), or some other parameter(s). We assume that there exist *scaling functions* $\gamma(x)$ and $\rho(x)$ satisfying

$$|\nabla\gamma| \le \frac{1}{2}, \qquad |x-y| \le \gamma(y) \implies c^{-1} \le \rho(x)/\rho(y) \le c, \tag{3.1.13$_{1,2}$}$$

such that after rescaling $x \mapsto x/\gamma(y)$ and $\xi \mapsto \xi/\rho(y)$ in $B(y,\gamma(y))$, we find ourselves in the framework of the previous chapter with an *effective semiclassical parameter* $\hbar \le 1$ [29].

To avoid non-degeneracy assumptions, we consider only the Schrödinger operator (2.70) in $\mathbb{R}^d$, assuming that $g^{jk} = g^{kj}$,

$$|\nabla^\alpha g^{jk}| \le c_\alpha \gamma^{-|\alpha|}, \qquad |\nabla^\alpha V| \le c_\alpha \rho^2 \gamma^{-|\alpha|} \tag{3.14}$$

and

$$\sum_{j,k} g^{jk}\xi_j\xi_k \ge \epsilon_0 |\xi|^2 \qquad \forall x,\xi. \tag{3.15}$$

In the examples below, $h \asymp 1$.

Example 3.2. (i) Suppose the conditions (3.14), (3.15) are fulfilled with $\gamma(x) = \frac{1}{2}(|x|+1)$ and $\rho(x) = |x|^m$, $m > 0$. Further, assume that the *coercivity condition*

$$V(x) \ge \epsilon_0 \rho^2 \tag{3.16}$$

holds for $|x| \ge c_0$. Then if $|x| \le C\lambda^{1/2m}$, for the operator $H-\lambda$, we can use $\rho_\lambda(x) = \lambda^{1/2}$ and then the contribution of the ball $B(x,\gamma(x))$ to the remainder does not exceed $C\lambda^{(d-1)/2}\gamma^{d-1}(x)$; summation over these balls results in $O\bigl(\lambda^{(d-1)(m+1)/2m}\bigr)$.

[29] In purely semiclassical settings, $\hbar = h/\rho\gamma$ and we assume $\rho\gamma \ge h$.

On the other hand, if $|x| \le C\lambda^{\frac{1}{2m}}$, for the operator $H - \lambda$ we can use $\rho(x) = \gamma^m(x)$ but there the ellipticity condition is fulfilled and then the contribution of the ball $B(x, \gamma(x))$ to the remainder does not exceed $C\gamma^{-s}$; summation over these balls results in $o\bigl(\lambda^{(d-1)(m+1)/2m}\bigr)$. Then we arrive to

$$\mathsf{N}(\lambda) = c_0 h^{-d} \int (\lambda - V(x))_+^{\frac{d}{2}} + O\bigl(\lambda^{(d-1)(m+1)/2m}\bigr) \tag{3.17}$$

as $\lambda \to +\infty$. Obviously the main part of the asymptotics is $\asymp \lambda^{d(m+1)/2m}$.

(ii) Suppose instead $0 > m > -1$. We are interested in its eigenvalues tending to the bottom of the continuous spectrum (which is 0) from below. We no longer require the assumption (3.16).

We use the same $\gamma(x)$ but now $\rho_\lambda(x) = \gamma(x)^m$ for $|x| \le C|\lambda|^{1/2m}$. Then the contribution of the ball $B(x, \gamma(x))$ to the remainder does not exceed $C\gamma(x)^{(d-1)(m+1)}$; summation over these balls results in $O\bigl(|\lambda|^{(d-1)(m+1)/2m}\bigr)$.

On the other hand, if $|x| \ge C|\lambda|^{1/2m}$, for the operator $H - \lambda$ we can use $\rho_\lambda(x) = |\lambda|^{\frac{1}{2}}$, but there the ellipticity condition is fulfilled and then the contribution of the ball $B(x, \gamma(x))$ to the remainder does not exceed $C|\lambda|^{-s}\gamma^{d-s}$; summation over these balls results in $o\bigl(|\lambda|^{(d-1)(m+1)/2m}\bigr)$. Then we arrive to asymptotics (3.17) again as $\lambda \to -0$.

Obviously the main part of the asymptotics is $O(|\lambda|^{d(m+1)/2m})$ and under the assumption $V(x) \le -\epsilon\rho(x)^2$, in some cone it is $\asymp |\lambda|^{d(m+1)/2m}$.

(iii) In both cases (i) and (ii), the main contribution to the remainder is delivered by the zone $\{\varepsilon < |x||\lambda|^{-1/2m} < \varepsilon^{-1}\}$ and assuming that $g^{jk}(x)$ and $V(x)$ stabilize as $|x| \to +\infty$ to $g^{jk0}(x)$ and $V^0(x)$, positively homogeneous functions of degrees 0 and $2m$ respectively, and that the set of periodic trajectories of the Hamiltonian $\sum_{j,k} g^{jk}(x)\xi_j\xi_k + V^0(x)$ on energy level 1 in (i) or -1 in (ii) has measure 0, we can improve the remainder estimates to $o\bigl(|\lambda|^{(d-1)(m+1)/2m}\bigr)$.

Example 3.3. Consider the Dirac operator

$$H = \sum_{1 \le j \le d} \sigma_j D_j + M\sigma_0 + V(x), \tag{3.18}$$

where σ_j ($j = 0, \dots, d$) are Pauli matrices in the corresponding dimension and $M > 0$. Let $V(x) \to 0$ as $|x| \to \infty$. Then the essential spectrum of H

is $(-\infty, -M] \cup [M, \infty)$ and for V as in Example 3.2(ii), we can get similar results for the asymptotics of eigenvalues tending to $M - 0$ or $-M + 0$: so instead of $\mathsf{N}(\lambda)$, we consider $\mathsf{N}(0, M - \eta)$ or $\mathsf{N}(M + \eta, 0)$ with $\eta \to +0$.

Example 3.4. Consider the Schrödinger operator, either in a bounded domain $X \ni 0$ or in $\mathbb{R}^d$ like in Example 3.2(i) and assume that $g^{jk}(x)$ and $V(x)$ have a singularity at 0 satisfying there (3.14)–(3.16) with $\gamma(x) = |x|$ and $\rho(x) = |x|^m$ with $m < -1$.

Consider the asymptotics of eigenvalues tending to $+\infty$. As in Example 3.2(i), we take $\gamma(x) = \frac{1}{2}|x|$ and $\rho_\lambda(x) = \lambda^{1/2}$ for $|x| \geq \epsilon_0 \lambda^{1/2m}$ (then the contribution of $B(x, \gamma(x))$ to the remainder does not exceed $\lambda^{(d-1)/2}|x|^{d-1}$) and $\rho_\lambda(x) = |x|^m$ as $|x| \leq \epsilon_0 \lambda^{1/2m}$ (then due to the ellipticity the contribution of $B(x, \gamma(x))$ to the remainder does not exceed $\rho^{-s}\gamma^{-s-d}$). We conclude that the contribution of $B(0, \epsilon)$ to the remainder does not exceed $C\lambda^{(d-1)/2}\epsilon^{d-1}$ which means that this singularity does not prevent remainder estimate as good as $o(\lambda^{(d-1)/2})$. However, this singularity affects the principal part which should be defined as in (3.17).

Example 3.5. (i) When analyzing the asymptotics of the large eigenvalues, we can consider a potential that is either rapidly increasing (with $\rho = \exp(|x|^m)$, $\gamma(x) = |x|^{1-m}$, $m > 0$), or slowly increasing (with $\rho = (|\log x|)^m$, $\gamma(x) = |x|$, $m > 0$) which affects both the magnitude of the main part and the remainder estimate.

(ii) When analyzing the asymptotics of the eigenvalues tending to the bottom of the essential spectrum, we can consider a potential that is either rapidly decreasing (with $\rho = |x|^{-1}(\log|x|)^m$ with $m > 0$, $\gamma(x) = |x|$, $m > 0$) or slowly decreasing (with $\rho = (|\log x|)^m$, $\gamma(x) = |x|$, $m < 0$) which affects both the magnitude of the main part as well as the remainder estimate.

Remark 3.6. We can consider the same examples albeit assuming only that $h \in (0, 1)$; then the remainder estimate acquires the factor h^{-d+1}.

Singularities

Let us consider other types of singularities when there is *a singular zone* where after rescaling $\hbar \leq 1$ [29]. Still, it does not prevent us from using the approach described above to get an estimate from below for (3.11) or (3.12): we only need to decrease these expressions by inserting ψ $(0 \leq \psi \leq 1)$ that is supported in *the regular zone* (aka *the semiclassical zone*) defined by $\hbar \le 2\hbar_0$ after rescaling and equal to 1 for $\hbar \le \hbar_0$ and applying the rescaling technique there.

Let us discuss an estimate from above. If there was no regular zone at all, we would have no estimate from below at all but there could be some estimate from above of variational nature. The best known is the LCR (Lieb-Cwikel-Rosenblum) estimate

$$\mathsf{N}^-(0) \le Ch^{-d} \int V_-^{\frac{d}{2}}\,dx \tag{3.19}$$

for the Schrödinger operator with Dirichlet boundary conditions as $d \ge 3$. For $d = 2$, the estimate is marginally worse (see [Roz1] for the most general statement for arbitrary orders of operators and dimensions and [Shar] for the most general results for the Schrödinger operator in dimension 2).

It occurs that we can split our domain into an overlapping *regular zone* $\{x:\ \rho(x)\gamma(x) \ge h\}$ and a *singular zone* $\{x:\ \rho(x)\gamma(x) \le 3h\}$, then evaluate the contribution of the regular zone using the rescaling technique and the contribution of the singular zone by the variational estimate as if on the inner boundary of this zone (i.e. a part of its boundary which is not contained in ∂X) the Dirichlet boundary condition was imposed, and we add these two estimates:

$$\begin{aligned} - Ch^{1-d} &\int_{\{\rho\gamma\ge h,\, V\le\epsilon\rho^2\}} \rho^{d-1}\gamma^{-1}\sqrt{g}\,dx \\ &\le \mathsf{N}^-(0) - (2\pi)^{-d}\omega_d h^{-d} \int_{\{\rho\gamma\ge h\}} V_-^{d/2}\,dx \\ &\le Ch^{1-d} \int_{\{\rho\gamma\ge h,\, V\le\epsilon\rho^2\}} \rho^{d-1}\gamma^{-1}\,dx + Ch^{-d}\int_{\{\rho\gamma\le h,\, V\le\epsilon\rho^2\}} \rho^d\,dx. \end{aligned} \tag{3.20}$$

See Theorems 9.1.7 and 9.1.13 of [Ivr4] for more general statements. Further, similar statements could be proven for operators which are not semi-bounded (see Theorems 10.1.7 and 10.1.8 of [Ivr4]).

In particular, we have:

Example 3.7. (i) Let

$$\int \rho^{d-1}\gamma^{-1}\,dx < \infty. \tag{3.21}$$

Then,

$$\mathsf{N}^-(0) = (2\pi)^{-d}\omega_d h^{-d}\int V_-^{d/2}\sqrt{g}\,dx + O(h^{1-d}). \tag{3.22}$$

(ii) If in addition the standard non-periodicity condition is satisfied then

$$\mathsf{N}^-(0) = (2\pi)^{-d}\omega_d h^{-d}\int V_-^{d/2}\sqrt{g}\,dx - \frac{1}{4}(2\pi)^{1-d}\omega_{d-1}h^{1-d}\int V_-^{(d-1)/2}\,dS + o(h^{1-d}), \tag{3.23}$$

where dS is a corresponding density on ∂X.

Example 3.8. Consider the Dirichlet Laplacian in a domain X assuming that there exists scaling function $\gamma(x)$ such that (3.14) holds and

(3.24) For each $y \in X$, the connected component of $B(y,\gamma(x))\cap X$ containing y coincides with $\{x \in B(0,1), x_1 \le f(x')\}$, where $x' = (x_2,\dots,x_d)$ and

$$|\nabla^\alpha f| \le C_\alpha \gamma^{1-|\alpha|} \qquad \forall\alpha, \tag{3.25}$$

where we rotate the coordinate system if necessary[30].

(i) Then the principal part of asymptotics is

$$c_0\lambda^{\frac{d}{2}}h^{-d}\int_{\{x:\gamma(x)\ge\lambda^{-\frac{1}{2}}\}} dx \tag{3.26}$$

and the remainder does not exceed

$$C\lambda^{\frac{d-1}{2}}h^{1-d}\int_{\{x:\gamma(x)\ge\lambda^{-\frac{1}{2}}\}}\gamma(x)^{-1}\,dx + C\lambda^{\frac{d}{2}}h^{-d}\int_{\{x:\gamma(x)\le\lambda^{-\frac{1}{2}}\}} dx. \tag{3.27}$$

(ii) In particular, if

$$\int_X \gamma(x)^{-1}\,dx < \infty, \tag{3.28}$$

[30] It is precisely the condition that we need to impose on the boundary for the rescaling technique to work.

then the standard asymptotics with the remainder estimate $O(\lambda^{(d-1)/2}h^{1-d})$ hold. Moreover, under the standard condition (1.3), we arrive to the two-term asymptotics (1.2).

These conditions are satisfied for domains with vertices, edges and conical points. In fact, we may allow other singularities including outer and inner spikes and cuts.

Furthermore, these conditions are satisfied for unbounded domains with cusps (exits to infinity) provided these cusps are thin enough (basically having finite volume and area of the boundary).

(iii) These results hold under the Neumann or mixed Dirichlet-Neumann boundary condition, but then we need to assume that the domain satisfies the cone condition; for the two-term asymptotics, we also need to assume that the border between the parts of ∂X with the Dirichlet and Neumann boundary conditions has $(d-1)$-dimensional measure 0.

Example 3.9. (i) Suppose that the potential is singular at $0 \in X$ like $|x|^{2m}$ with $m \in (-1, 0)$. Then this singularity does not affect the asymptotics of large eigenvalues.

(ii) Let us consider Example 3.2(i) albeit allow $V \geq 0$ to vanish along certain directions. Then we have *canyons* and $\{x : V(x) \leq \lambda\}$ are cusps. If the canyons are narrow and steep enough then the same asymptotics (3.17) hold. Moreover, under the non-periodicity condition, the remainder estimate is "o".

(iii) Let us consider Example 3.2(ii) albeit allow $V \geq 0$ to be singular along certain directions. Then we have *gorges* and $\{X : V(x) \leq \lambda\}$ are cusps. If the gorges are narrow and shallow enough then the same asymptotic (3.17) hold. Moreover, under the non-periodicity condition, the remainder estimate is "o".

Example 3.10. We can consider also multiparameter asymptotics, for example with respect to $h \to +0$ and λ. In addition to what we considered above, the following interesting possibility appears: $\lambda \searrow \lambda_* := \inf V(x)$ which is either finite or $-\infty$. Then if λ tends to λ_* slowly enough so that $\mathsf{N}^-_h(\lambda) \to +\infty$, we get interesting asymptotics.

In particular, as either $V(x) \asymp |x|^{2m}$ with $m > 0$ and $\lambda \to +0$ or $V(x) \asymp |x|^{2m}$ with $0 > m > -1$ and $\lambda \to -\infty$, then this condition is $h = o(|\lambda|^{(m+1)/2m})$.

Remark 3.11. We can also consider $\mathsf{Tr}((-H)^\nu \theta(-H))$ with $\nu > 0$. Then in the estimates above, $\rho^d \mapsto \rho^{d+2\nu}$ and $\rho^{d-1} \mapsto \rho^{d+\nu-1}\gamma^{-\nu-1}$.

For full details, proofs and generalizations, see Chapter 11 of [Ivr4] which covers also non-semibounded operators.

Non-Weyl Asymptotics

Partially Weyl Theory

Analyzing the examples of the previous section, one can observe that for some values of the exponents, the condition (3.21) (or it special case (3.28)) fails but the main term of the asymptotics is still finite and has the same rate of the growth as it had before, while for other values of the exponent, it is infinite. In the former case, we get Weyl asymptotics but with a worse remainder estimate, in the latter case, all we can get is an estimate rather than the asymptotics. Can one save the day?

In many cases, the answer is positive and we can derive either the Weyl asymptotics but with a non-Weyl correction term or completely non-Weyl asymptotics. The main but not the only tool is the spectral asymptotics for operators with operator-valued symbols. Namely, in some zone of the phase space, we separate the variables[31] $x = (x'; x'')$ and $(\xi'; \xi'')$ respectively and consider the variables (x', ξ') as *semiclassical variables* (or *Weyl variables*), similar to (x, ξ) in the previous scheme. So we get an operator $\mathsf{H}(x', D')$ with an operator-valued symbol which we can study in the same way as the operator H before.

One can say that we have a matrix operator but with a twist: first, instead of finite-dimensional matrices, we have unbounded self-adjoint operators in the auxilary infinite-dimensional Hilbert space $\mathbb{H}$ (usually $\mathscr{L}^2$ in the variables x''); second, we are interested in the asymptotics

$$\int \mathrm{tr}_{\mathbb{H}}\big(\hat{e}(x', x', \lambda)\big)\, dx', \tag{3.29}$$

[31] After some transformation, the transformations and separations in the different zones are not necessarily the same.

rather than in the asymptotics without trace where $\hat{e}(x',y';\lambda)$ is an operator in $\mathbb{H}$ (with Schwartz kernel $e(x',y';x'',y'';\lambda)$); and, finally, the main term in asymptotics is

$$\int \mathsf{tr}_{\mathbb{H}}\bigl(\mathsf{e}(x',\xi';\lambda)\bigr)\,d\xi' dx', \tag{3.30}$$

where $\mathsf{e}(x',\xi',\lambda)$ is a spectral projector (in $\mathbb{H}$) of $\mathsf{H}(x',\xi')$. Here, we need to assume that $\mathsf{H}(x',\xi')$ is microhyperbolic with respect to (x',ξ'). Since the operator $\mathsf{tr}_{\mathbb{H}}$ is now unbounded, both the main term of the asymptotics of (3.29) and the remainder estimate *may* have magnitudes different from what they would be without $\mathsf{tr}_{\mathbb{H}}$.

Since the operator $\mathsf{H}(x',\xi')$ is rather complicated, we want to replace it by some simpler operator and add some easy to calculate correction terms.

We consider multiple examples below. Magnetic Schrödinger, Schrödinger-Pauli and Dirac operators studied in Sections 2 and 3 are also of this type.

Domains with Thick Cusps

This was done in Section 12.2 of [Ivr4] for operators in domains with thick cusps of the form $\{x:\ x''\in f(x')\Omega\}$ where Ω is a bounded domain in $\mathbb{R}^{d''}$ with smooth boundary, defining the cusp crossection. Here again we consider for simplicity the Dirichlet Laplacian. Assume first that the metric is Euclidean and the domain $X=\{x=(x',x''):\ x'\in X':=\mathbb{R}^{d'},\ x''\in f(x')\Omega\}$. Then, the change of variables $x''\mapsto x''/f(x')$ transforms Δ to the operator

$$P=\sum_{1\le j\le d'}\Bigl(D_j+g_{x_j}L+\frac{id''}{2}g_{x_j}\Bigr)\Bigl(D_j+g_{x_j}L-\frac{id''}{2}g_{x_j}\Bigr)+\frac{1}{f^2}\Delta'' \tag{3.31}$$

in $\mathscr{L}^2(X'\times\Omega)=\mathscr{L}^2(\mathbb{R}^{d'},\mathbb{H})$ where $L=\langle x'',D''\rangle$, $g=-\log f$, $\mathbb{H}=\mathscr{L}^2(\Omega)$, Δ' is a Laplacian in X', and $\Delta''=\Delta''_{\mathsf{D}}$ is a Dirichlet Laplacians in Ω, and we simultaneously multiply u by $f^{-d''/2}$ to have the standard Euclidean measure rather than the weighted one $f^{d''}dx$. We consider the operator (3.31) as a perturbation of the operator

$$\bar{P}:=\Delta'+\frac{1}{f^2}\Delta'', \tag{3.32}$$

which is a direct sum of d'-dimensional Schrödinger operators $P_n=\Delta'+\mu_n f^{-2}$ in X' where $\mu_n>0$ are the eigenvalues of Δ''_{D}. Assuming that

$$f\asymp |x|^{-m},\qquad |\nabla f|\asymp |x|^{-m-1}\qquad \text{for}\ \ |x'|\ge c, \tag{3.33}$$

we can ensure that the microhyperbolicity condition (with respect to $(x';\xi')$) is fulfilled for P_n, $\bar{P}$, as well as for P.

Then according to the previous section, for P_n the eigenvalue counting function is

$$\text{(3.34)}\quad \mathsf{N}_n(\lambda) = c_{d'}\int \bigl(\lambda-\mu_n f^{-2}(x')\bigr)_+^{\frac{d'}{2}}\,dx' + O\bigl(\lambda^{(d'-1)(m+1)/2m}\mu_n^{-(d'-1)/2m}\bigr),$$

where the remainder estimate is uniform with respect to n. Observe that for $\bar{P}$ the eigenvalue counting function is $\bar{\mathsf{N}}(\lambda)=\sum_n \mathsf{N}_n(\lambda)$. Using $\mu_n \asymp n^{2/d''}$, we arrive to

$$\text{(3.35)}\qquad \mathsf{N}_n(\lambda) = c_{d'}\iint (\lambda-\mu f^{-2}(x'))_+^{\frac{d'}{2}}\,dx'd_\mu \boldsymbol{n}(\mu) + O(R(\lambda))$$

with

$$\text{(3.36)}\qquad R(\lambda)=\lambda^{\frac{1}{2}(d-1)}+\lambda^{\frac{m+1}{2m}(d'-1)}+\delta_{(d'-1),md''}\lambda^{\frac{1}{2}(d-1)}\log\lambda,$$

where $\boldsymbol{n}(\mu)$ is the eigenvalue counting function for Δ''_{D}.

We show, moreover, that the same asymptotics holds for our original operator (3.31). Furthermore, if the first term in (3.35) is dominant, then under the standard non-periodicity assumption we can replace $O(\lambda^{(d-1)/2})$ by $o(\lambda^{(d-1)/2})$; we need to add the standard boundary term to the right-hand expression in (3.35).

On the other hand, if the second term in (3.35) dominates, then assuming that f stabilizes as $|x'|\to\infty$ to a positively homogeneous function f_0, under the corresponding non-periodicity assumption (now in $T^*\mathbb{R}^{d'}$) for $|\xi'|^2+f_0^{-2}(x')$, we can replace $O(\lambda^{(m+1)(d'-1)/2m})$ by $o(\lambda^{(m+1)(d'-1)/2m})$. Finally, if both powers coincide then under the stabilization condition, the remainder estimate is $o(\lambda^{(d-1)/2}\log\lambda)$ but we need to add the modified boundary term to the right-hand expression in (3.35).

Obviously, the principal part in (3.35) is of the magnitude

$$\text{(3.37)}\qquad S(\lambda)=\lambda^{\frac{1}{2}d}+\lambda^{\frac{m+1}{2m}d'}+\delta_{d',md''}\lambda^{\frac{1}{2}d}\log\lambda.$$

If X is not exactly of the same form and the metric only stabilizes (fast enough) at infinity to $g^{jk0}:=\delta_{jk}$, then we can recover the same remainder estimate and reduce the principal part to

$$\text{(3.38)}\quad c_{d'}\iint (\lambda-\mu f^{-2}(x'))_+^{\frac{d'}{2}}\phi(x')\,dx'd_\mu\boldsymbol{n}(\mu) \\ + c_d\lambda^{d/2}\int_X (\sqrt{g}-\sqrt{g^0}\phi(x'))\,dx,$$

where $\mathsf{supp}(\phi) \subset \{|x'| \geq c\}$, $\phi = 1$ in $\{|x'| \geq c\}$. Here, the first part is exactly as above and the second term is actually the sum of two terms; one of them $c_d\lambda^{d/2}\int \sqrt{g}(1-\phi(x'))\,dx$ is the contribution of the "finite part of the domain" (without the cusp) and the second $c_d\lambda^{d/2}\int(\sqrt{g}-\sqrt{g^0})\phi(x')\,dx$ is a contribution of the cusp in the correction.

Note that now to get the remainder estimate $o(\lambda^{(d-1)/2})$, one needs to include the standard boundary term in the second part of (3.38).

The crucial part of our arguments is a *multiscale analysis*. As long as $r \leq c\lambda^{1/2m-\delta}$, we can scale $x \mapsto xr^m$ and consider $\sigma_0(t) = \mathsf{Tr}\bigl(e^{ih^{-1}tH}\phi(x'/r)\bigr)$; here $H = \lambda^{-1}P$, $h = \lambda^{-1/2}r^m$. From the propagation with respect to (x,ξ), we know that on energy level 1, the time interval $(h^{1-\delta},\epsilon)$ contains no singularities of $\sigma_0(t)$.

On the other hand, for $r \geq c$, we can scale $x \mapsto x/r$ and consider $\sigma_1(t) = \mathsf{Tr}\bigl(e^{i\hbar^{-1}tH}\phi(x'/r)\bigr)$; here $\hbar = \lambda^{-1/2}r^{-1}$. From the propagation with respect to (x',ξ'), we know that on energy level 1, the time interval $(\hbar^{1-\delta},\epsilon)$ contains no singularities of $\sigma_1(t)$.

Observe first that $\sigma_1(t) = \sigma_0(r^{-1-m}t)$ and therefore the time interval $(h^{1-\delta},\epsilon r^{m+1})$ contains no singularities of $\sigma_0(t)$. This allows us to improve the remainder estimate in the full Weyl asymptotics but we need to include many terms which are difficult to calculate.

On the other hand, for $\lambda^\delta \leq r \leq c\lambda^{1/2m}$, we can consider H as a perturbation of $\bar{H} = \lambda^{-1}\bar{P}$. We do it first in the framework of the theory of operators with operator-valued symbols. Then we consider all perturbation terms and apply to them "full Weyl theory" and due to the stabilization assumption, the error is less than (3.36). This gives us another asymptotics, also with many terms which are difficult to calculate.

Comparing these two asymptotics in their common domain $\lambda^\delta \leq r \leq \lambda^{1/2m-\delta}$, we conclude that all terms but those present in both must be 0; it allows us to eliminate almost all the terms and sew these asymptotics resulting in (3.38).

Using the same approach, we can consider higher order operators, the case when X' is a conical set and there are several cusps X_k which may have different dimensions d'_k and rates of decay (then both the principal part and the remainder estimate should be modified accordingly).

Neumann Laplacian in Domains with Ultra-Thin Cusps

Consider the Neumann Laplacian in domains with cusps. Recall that since these domains do not satisfy the cone condition, we so far have no results even if the cusp is thin. Applying the same arguments as before, we hit two obstacles. The first (minor) obstacle is that the Neumann boundary condition for the operator (3.31) coincides with the same condition for Δ'' only asymptotically. The second (major) obstacle is that $\mu_1 = 0$ and $P_1 = \Delta'$ has a continuous spectrum. In fact, we should not reduce P to $\bar{P}$; from (3.31) we conclude that

$$P_1 = \sum_{1\le j\le d'} \Bigl(D_j + \frac{id''}{2} g_{x_j}\Bigr)\Bigl(D_j - \frac{id''}{2} g_{x_j}\Bigr) = \Delta' + W \tag{3.39}$$

with

$$W = \frac{d''^2}{4}|\nabla g|^2 + \frac{d''}{2}\Delta' g. \tag{3.40}$$

Still this operator may have a continuous spectrum unless $|\nabla g| \to \infty$ as $|x| \to \infty$. We need to assume that f has superexponential decay: $f = e^{-g}$ with

$$|\nabla^\alpha g| \le c_\alpha |x|^{1+m-|\alpha|} \qquad \forall \alpha, \tag{3.41}$$

$$g \asymp |x'|^{m+1}, \quad |\nabla g| \asymp |x'|^m \qquad \text{for } |x'| \ge c, \tag{3.42}$$

$$|\nabla |\nabla g|^2| \asymp |x|^{2m-1} \qquad \text{for } |x'| \ge c, \tag{3.43}$$

where $m > 0$ and (3.43) is a microhyperbolicity condition for P_1. Then one can prove easily that when $d'' \ge 2$,

$$\mathsf{N}(\lambda) = c_d \lambda^{d/2} \int_X \sqrt{g}\, dx + c_{d'} \int (\lambda - W)_+^{d'/2}\, dx' + O(R(\lambda)) \tag{3.44}$$

with

$$R(\lambda) = \lambda^{\frac{1}{2}(d-1)} + \lambda^{\frac{m+1}{2m}(d'-1)}. \tag{3.45}$$

Moreover, if the first term in (3.35) dominates, then under the standard non-periodicity assumption, we can replace $O(\lambda^{(d-1)/2})$ by $o(\lambda^{(d-1)/2})$ (simultaneously including the standard boundary term); if the second term dominates, then assuming that W stabilizes as $|x'| \to \infty$ to a positively homogeneous function W_0, under the corresponding assumption for $|\xi'|^2 + W_0(x')$ we can replace $O(\lambda^{(m+1)(d'-1)/2m})$ by $o(\lambda^{(m+1)(d'-1)/2m})$.

One can see easily that $\mathsf{N}(\lambda) \asymp S(\lambda) = \lambda^{\frac{1}{2}d} + \lambda^{\frac{m+1}{2m}d'}$. Observe that in contrast to (3.36) and (3.37), even if the exponents coincide, a logarithmic factor does not appear.

The case $d''=1$ is special since even an ultra-thin cusp is also thick (according to the classification of the previous Subsection 3) and the corresponding formulae should include a modified boundary term containing the double logarithm of λ. For this and other generalizations, see Section 12.7 of [Ivr4]. Also one can consider *spikes* with $\operatorname{supp}(f) = \{|x'| \le L\}$, in which case the standard Weyl asymptotics holds.

Operators in $\mathbb{R}^d$

The scheme of Subsection 3 is repeated in many similar cases.

First, consider eigenvalues tending to $+\infty$ for the Schrödinger operator with potential V which generically is $\asymp |x|^{2m}$ but vanishes along some directions.

For example, consider the toy-model $V = |x|^{2m-2m'}|x''|^{2m'}$ with $m > m' > 0$. Let $X' = \mathbb{R}^{d'} \ni x'$ and $X'' = \mathbb{R}^{d''} \ni x''$. Consider only the conical vicinity of X' and here we instead consider the potential $V = |x'|^{2m-2m'}|x''|^{2m'}$. Consider only the part of operator which is related to x'': $\Delta'' + |x'|^{2m-2m'}|x''|^{2m'}$ and after the change of variables $x'' \mapsto x''|x'|^k$ with $k = (m-m')/(m'+1)$, it becomes $|x'|^{2k}L$ with $L = \Delta'' + U(x'')$, $U = |x''|^{2m''}$. The condition $m''>0$ ensures that the spectrum of L is discrete and accummulates to $+\infty$.

So basically we have a mixture of the Schrödinger operator on $\mathbb{R}^d$ with a potential growing as $|x|^{2m}$ and the Schrödinger operator with the operator-valued symbol on $\mathbb{R}^{d''}$ with a potential growing as $|x|^{2k}$ and we recover the asymptotics with the remainder estimate $O(R(\lambda))$, where

$$R(\lambda) = \lambda^{\frac{m(d-1)}{(m+1)}} + \lambda^{\frac{k(d'-1)}{(k+1)}} + \delta_{\frac{m(d-1)}{(m+1)},\frac{k(d'-1)}{(k+1)}}\lambda^{\frac{m(d-1)}{(m+1)}}\log\lambda \tag{3.46}$$

and the principal part is $\asymp S(\lambda)$, where

$$S(\lambda) = \lambda^{\frac{md}{(m+1)}} + \lambda^{\frac{kd'}{(k+1)}} + \delta_{\frac{md/(m+1)}{,}\frac{kd'}{(k+1)}}\lambda^{\frac{md}{(m+1)}}\log\lambda. \tag{3.47}$$

In a rather general situation, this principal part is similar to the one in (3.38) where $\boldsymbol{n}(\mu)$ is the eigenvalue counting function for L. Further, under similar non-periodicity assumptions, we can replace "O" by "o". For generalizations, details and proofs, see Section 12.3 of [Ivr4].

Second, consider eigenvalues tending to -0 for the Schrödinger operator with a potential V which generically is $\asymp |x|^{2m}$ with $m \in (-1,0)$ but is singular in some directions. Again, consider a toy-model $V = -|x|^{2m-2m'}|x''|^{2m'}$ with $-1 < m < m' < 0$. Again, $L = \Delta'' + U(x'')$, $U = -|x''|^{2m''}$ and its negative spectrum is discrete and accummulates to -0. The formulae (3.46) and (3.47) remain valid (albeit $\lambda \to -0$). For generalizations, details and proofs, see Section 12.4 of [Ivr4].

Maximally Hypoelliptic Operators

Third, consider the eigenvalues tending to $+\infty$ for *maximally hypoelliptic operators with a symplectic manifold of degeneration*. Consider the toy-model $P = \Delta'' + |x''|^{2m}\Delta'$. In this case, after the partial Fourier transform, we get $\Delta'' + |x''|^{2m}|\xi'|^2$ and after the change of variables $x'' \mapsto |\xi'|^k x''$, we get $|\xi'|^{2k}L$, $L = \Delta'' + |x''|^{2m}$ and $k = 1/(m+1)$.

This toy-model is maximally hypoelliptic as the spectrum of L is discrete and accummulates to $+\infty$. So basically we have a blend of operator of order 2 on $\mathbb{R}^d$ and of order $2k$ on $\mathbb{R}^{d'}$ and we recover the asymptotics with remainder estimate $O(R(\lambda))$ with

$$R(\lambda) = \lambda^{\frac{(d-1)}{2}} + \lambda^{\frac{(d'-1)}{2k}} + \delta_{d-1,(d'-1)/k}\lambda^{\frac{(d-1)}{2}}\log\lambda \tag{3.48}$$

and principal part $\asymp S(\lambda)$ with

$$S(\lambda) = \lambda^{\frac{d}{2}} + \lambda^{\frac{d'}{2k}} + \delta_{d,d'/k}\lambda^{\frac{d}{2}}\log\lambda. \tag{3.49}$$

Further, under similar non-periodicity assumptions, we can replace "O" by "o". For generalizations, details and proofs, see Section 12.5 of [Ivr4].

Trace Asymptotics for Operators with Singularities

Here, we also consider only one example (albeit the most interesting one) of a Schrödinger operator $H := h^2\Delta - V(x)$ in $\mathbb{R}^3$ with potential $V(x)$ at 0 stabilizing to a positive homogeneous function V_0 of degree -1:

$$|\nabla^\alpha(V - V_0)| \le c_\alpha |x|^{-|\alpha|} \qquad \forall\alpha. \tag{3.50}$$

We assume that $V(x)$ decays fast enough at infinity and we are interested in the asymptotics of $\mathsf{Tr}(H_-)$, which is the sum of the negative eigenvalues of H. While generalizations are considered in Section 12.6 of [Ivr4], exactly this problem with $V_0 = |x|^{-1}$ arises in the asymptotics of the ground state energy of heavy atoms and molecules.

It follows from Section 3 that N_h^- has purely Weyl asymptotics with the remainder estimate $O(h^{-2})$ and[32] it could be improved to $o(h^{-2})$ but we have a different object and if the potential had no singularities, the remainder estimate would be $O(h^{-1})$ or even $o(h^{-1})$[32),33)].

Therefore considering the contribution of the ball $B(x,\gamma(x))$ with $\gamma(x) = \frac{1}{2}|x|$, we have a contribution to the Weyl expression

$$-ch^{-3}\int V_+^{\frac{5}{2}}\,dx \tag{3.51}$$

of magnitude $C\rho^2(h/\rho\gamma)^{-3} = Ch^{-3}\rho^5\gamma^3$, while the contribution to the remainder does not exceed $C\rho^2(h/\rho\gamma)^{-1} = Ch^{-1}\rho\gamma$ with $\rho = |x|^{-\frac{1}{2}}$. We see that the former converges at 0 and the latter diverges. This analysis could be done for $\rho\gamma \ge h$ i.e. if $|x| \ge h^2$. Then we conclude that the contribution of the zone $\{x:\ |x| \ge a\}$ to the remainder does not exceed $Ch^{-1}a^{-\frac{1}{2}}$ which as $a = h^2$ is $O(h^{-2})$. On the other hand, one can easily prove that the contribution of $B(0,h^2)$ to the asymptotics is also $O(h^{-2})$.

To improve this estimate, we analyze $B(0,a)$ in more detail. In virtue of (3.50), we can easily prove that the contribution of $B(x,\gamma)$ to $\mathsf{Tr}(H_- - H_{0-})$ (with $H_0 = h^2\Delta - V_0$) does not exceed $C(h/\rho\gamma)^{-2} = Ch^{-2}\rho^2\gamma^2$ and therefore the contribution of $B(0,a)$ to the remainder is $O(h^{-2}a)$. Minimizing the total error $h^{-2}a + h^{-1}a^{-\frac{1}{2}}$ in a, we get $a = h^{\frac{2}{3}}$ and the remainder $O(h^{-\frac{4}{3}})$, which is better than $O(h^{-2})$ but not as good as $O(h^{-1})$.

But then we need to include in the asymptotics the extra term

$$\int \bigl(e_0^1(x,x,0) - cV_+^{\frac{5}{2}}(x)\bigr)\psi(a^{-1}x)\,dx, \tag{3.52}$$

where $e(\cdot,\cdot,\lambda)$ is the Schwartz kernel of the spectral projectors for H, $e^1(\cdot,\cdot,0) = \int_{-\infty}^0 \lambda\, d_\lambda e(\cdot,\cdot,\lambda)$ and the subscript 0 means that it is for H_0 and $\psi \in \mathscr{C}_0^\infty(B(0,2))$ and equals 1 in $B(0,1)$.

[32] Under the standard non-periodicity condition.

[33] But then the principal part of asymptotics should include the third term ch^{-1} while the second term vanishes.

Basically, all that we achieved so far was to replace H by H_0 in (3.52). The same arguments allow us to replace ψ by 1 in this expression with the same error $O(h^{-1}a^{-\frac{1}{2}})$. This time, we cannot decompose it as the difference of two integrals because each of them is diverging at infinity (since V_0 decays there not fast enough). Further, due to the homogeneity of V_0, one can prove that this remodelled expression (3.52) is homogeneous of degree -2 with respect to h and thus is equal to κh^{-2}. Here, κ is some unknown constant, but for $V_0 = |x|^{-1}$, it could be calculated explicitly.

Therefore, we conclude that with the remainder estimate $O(h^{-\frac{4}{3}})$, $\mathrm{Tr}(H_-)$ is given by the Weyl expression plus the *Scott corretion term* κh^{-2}.

To improve this remainder estimate, we should carefully study the propagation of singularities. We can prove that if $h^{2-\delta} \le \gamma \le 1$, then the singularities do not come back "in real time" $\asymp 1$, which is a vast improvement over $\asymp \gamma\rho^{-1} \asymp \gamma^{\frac{3}{2}}$. Then the contribution of $B(x,\gamma)$ to the "trace remainder" does not exceed $Ch^{-1}\rho^2\gamma^3$ but then the principal part of asymptotics should have a lot of terms; the n-th term is of the magnitude $h^{-3+2n}\rho^{2-2n}\gamma^{3-2n}$; however, using (3.50) we conclude that the difference between such terms for H and H_0 is $O(h^{-3+2n}\rho^{-2n}\gamma^{3-2n})$ which leads to the estimate

$$\left| \int \left(e^1(x,x,0) - e^1_0(x,x,0) - cV_+^{\frac{5}{2}}(x) + cV_{0+}^{\frac{5}{2}}(x) \right) dx \right| \le Ch^{-1}. \tag{3.53}$$

This estimate implies that with the remainder estimate $O(h^{-1})$, $\mathrm{Tr}(H_-)$ is given by the Weyl expression plus κh^{-2}. Moreover, this estimate could be further improved to $o(h^{-1})$ [32),33)].

Similar results hold for other singularities (including singularities of the boundary), dimensions and $\mathrm{Tr}(H_-^\nu)$ with $\nu > 0$. However, note that there could be more than one such correction term.

Periodic Operators

Finally, consider an operator $H_0 = H_0(x, D)$ with periodic coefficients (with the lattice of periods Γ). Then its spectrum is usually absolutely continuous and consists of *spectral bands* $\{\lambda_k(\xi) : \xi \in \mathcal{Q}'\}$ separated by *spectral gaps*. Here, λ_k are the eigenvalues of operator H_0 with *quasiperiodic boundary conditions*

$$u(x+n) = T^n e^{i\langle n,\xi\rangle}(x) \qquad \forall n \in \Gamma, \tag{3.54}$$

Γ^* is the dual lattice[34)], $\mathcal{Q}$ and $\mathcal{Q}'$ are corresponding *elementary cells*[35)]; ξ is called the *quasimomentum*. Here, $T = (T_1, \dots, T_d)$ is a family of commuting unitary matrices.

Let us consider an operator $H_t = H_0 - tW(x)$ with $W(x) > 0$ decaying at infinity. Then, while the essential spectra of H and H_t are the same, H_t can have discrete eigenvalues in the spectral gaps and these eigenvalues decrease as t increases.

Let us fix an *observation point* E belonging to either the spectral gap or its boundary and introduce $\mathsf{N}_E(\tau)$, the number of eigenvalues of H_t crossing E as t changes between 0 and τ. We are interested in the asymptotics of $\mathsf{N}_E(\tau)$ as $t \to \infty$.

Then using Gelfand's transform,

$$\mathcal{F}u(\xi, x) = (2\pi)^{\frac{d}{2}} (\operatorname{vol}(\mathcal{Q}'))^{-1} \sum_{n\in\Gamma} T^n e^{-i\langle n-x,\xi\rangle} u(x-n) \tag{3.55}$$

with $(x, \xi) \in \mathcal{Q} \times \mathcal{Q}'$, this problem is reduced to the problem for operators with operator-valued symbols on $\mathscr{L}^2(\mathcal{Q}', \mathbb{H}_{\xi,\{T\}})$ where $\mathbb{H}_{\xi,\{T\}}$ is the space of functions satisfying (3.54).

After that, different results are obtained in three essentially different cases: when E belongs to the spectral gap, E belongs to the bottom of the spectral gap, and E belongs to the top of the spectral gap. For exact results, proofs and generalizations, see Section 12.8 of [Ivr4].

4 Non-Smooth Theory

So far we have considered operators with smooth symbols in domains with smooth boundaries. Singularities were possible but only on "lean" sets. However, it turns out that many results remain true under very modest smoothness assumptions.

Non-Smooth Symbols and Rough Microlocal Analysis

To deal with non-smooth symbols, we approximate them by *rough* symbols $p \sim \sum_m p_m$, depending on a small *mollification parameter* ε and satisfying

$$|\nabla_\xi^\alpha \nabla_x^\beta p_m(x,\xi)| \le C_{m\alpha\beta} \boldsymbol{\rho}^{-\alpha} \boldsymbol{\gamma}^{-\beta} \varepsilon^{-m} \tag{1.1}$$

34) I.e. if $\Gamma = \mathbb{Z}e_1 \oplus \mathbb{Z}e\_2 \oplus \dots \oplus \mathbb{Z}e_d$ then $\Gamma^* = \mathbb{Z}e'_1 \oplus \mathbb{Z}e'_2 \oplus \dots \oplus \mathbb{Z}e'_d$ with $\langle e_j, e'_k\rangle = \delta_{jk}$.

35) I.e. $\mathcal{Q} = \{x_1e_1 + \dots + x_de_d :\ x \in [0,1]^d\}$ and $\mathcal{Q}'* = \{\xi_1e'_1 + \dots + \xi_de'_d :\ \xi \in [0,1]^d\}$.

with

$$\min_j \rho_j\gamma_j \ge \varepsilon \ge Ch^{1-\delta} \tag{1.2}$$

(*microlocal uncertainty principle*), which could be weakened to

$$|\nabla_\xi^\alpha \nabla_x^\beta p_m(x,\xi)| \le C^{|\alpha|+|\beta|+m+1}\alpha!\beta!m!\boldsymbol{\rho}^{-\alpha}\boldsymbol{\gamma}^{-\beta}\varepsilon^{-m} \qquad \forall \alpha,\beta,m : |\alpha|+|\beta|+2m \le N = C|\log h|^{-1} \tag{1.3}$$

with

$$\min_j \rho_j\gamma_j \ge \varepsilon \ge Ch|\log h| \tag{1.4}$$

(*logarithmic uncertainty principle*). At this point, microlocal analysis ends: the assumptions cannot be weakened any further.

Assuming that

$$|\nabla_\xi^\alpha \nabla_x^\beta \nabla p_0(x,\xi)| \le C^{|\alpha|+|\beta|+1}\alpha!\beta!\boldsymbol{\rho}^{-\alpha}\boldsymbol{\gamma}^{-\beta} \tag{1.5}$$

and

$$|\nabla_\xi^\alpha \nabla_x^\beta \nabla p_m(x,\xi)| \le C^{|\alpha|+|\beta|+m+1}\alpha!\beta!m!\boldsymbol{\rho}^{-\alpha}\boldsymbol{\gamma}^{-\beta}\varepsilon^{1-m} \quad (m\ge 1), \tag{1.6}$$

we can restore Theorem 2.2 (see Theorem 2.3.2 of [Ivr4]) and therefore also the Corollaries 2.3 and 2.4, assuming ξ-microhyperbolicity instead of the usual microhyperbolicity. For proofs and details, see Section 2.3 of [Ivr4].

After this, we can than use the successive approximation method like in Subsection 2 (definitely some extra twisting required) and then recover the spectral asymptotics – originally only for operators which are ξ-microhyperbolic.

To consider non-smooth symbols, we can bracket them between rough symbols: for example, for the Schrödinger operator $p^-(x,\xi,h) \le p(x,\xi,h) \le p^+(x,\xi,h)$ where $p^\pm = p_\varepsilon \pm C\nu(\varepsilon)$ and p_ε is the symbol p, ε-mollified and $\nu(\varepsilon)$ is the modulus of continuity of the metric and potential; $\varepsilon = Ch|\log h|$.

Then for $\nu(\varepsilon) = O(\varepsilon|\log\varepsilon|^{-1})$ [36], we can recover the remainder estimate $O(h^{1-d})$; under even weaker regularity conditions by rescaling, we can recover weaker remainder estimates. On the other hand, if $\nu(\varepsilon) = o(\varepsilon|\log\varepsilon|^{-1})$,

[36] Which means that the first partial derivatives are continuous with modulus of continuity $\nu_1(\varepsilon) = \nu(\varepsilon)\varepsilon^{-1}$.

we can recover the remainder estimate $o(h^{1-d})$ under the standard non-periodicity condition[37)]. For proofs and details, see Section 4.6 of [Ivr4]. There is an alternative to the bracketing construction based on perturbation theory, which works better for the trace asymptotics and also covers the pointwise asymptotics. For an exposition, see Section 4.6 of [Ivr4].

Further, for scalar and similar operators, the rescaling technique allows us to replace ξ-microhyperbolicity by microhyperbolicity under really weak smoothness assumptions; here we also use ε depending on the point so that we can consider scalar symbols under weaker and weaker non-degeneracy assumptions albeit stronger and stronger smoothness assumptions. See Section 5.4 of [Ivr4].

Non-Smooth Boundaries

Let us consider a domain with non-smooth boundary (with the Dirichlet boundary condition). Here, the standard trick to flatten out the boundary by the change of variables $x_1 \mapsto x_1 - \phi(x')$ works very poorly: the operator principal symbol contains the first partial derivatives ϕ and therefore we need to require $\phi \in \mathscr{C}^2$. Fortunately, the method of R. Seelley [See1] can help us. This method was originally developed for the Laplacian with a smooth metric and a smooth boundary.

Here, we consider only the Schrödinger operator; assume first that the metric and potential are smooth. Consider a point $\bar{x} \in X$ and assume that the metric is Euclidean at $\bar{x}$ and nearby, X looks like $\{x : x_1 \geq \phi(x')\}$ with $\nabla'\phi(\bar{x'}) = 0$. Observe that these assumptions do not require any smoothness beyond $\mathscr{C}^1$.

Consider a trajectory starting from $(\bar{x}, \xi)$. If $|\xi_1| < \rho := Ch|\log h|/\gamma$, the trajectory starts parallel to ∂X and ∂X can "catch up" only at time at least $T = \sigma(\gamma)$ where $\gamma = \frac{1}{2}\mathsf{dist}(x, \partial X)$ and σ is the inverse function to ν, which is a modulus of continuity for ϕ[36)].

If $\xi_1 > \rho$ then this trajectory "runs away from ∂X" and ∂X can "catch up" only at time at least $T = \sigma(\gamma) + \sigma_1(\xi_1)$ where σ_1 is the inverse function to ν_1[36)]. On the other hand, if $\xi_1 < -\rho$, then we can revert the trajectory (which works only for local but not pointwise spectral asymptotics).

[37)] However, even for the Schrödinger operator without boundary, the dynamic equations do not satisfy the Lipschitz condition and thus the flow could be multivalued.

These arguments allow us to estimate the contribution of $B(x, \gamma(x))$ to the remainder by $Ch^{1-d}\gamma^d h|\log h|\sigma(\gamma)^{-1}$ and then the total remainder by $Ch^{1-d}\int \sigma(\gamma)^{-1}\,dx$. The latter integral converges for $\nu(t) = t|\log t|^{-1-\delta}$.

Sure, this works only when $\gamma \geq \bar\gamma = Ch|\log h|$. However, if we smoothen the boundary with a smoothing parameter $C\bar\gamma$, for $\gamma \leq \bar\gamma$, we will be in the framework of the smooth theory after rescaling and we can take $T = \bar\gamma$. The contribution of this strip to the remainder does not exceed $Ch^{1-d}\bar\gamma T^{-1}$ as its measure does not exceed $C\bar\gamma$. One can easily check that the variation of $\mathsf{vol}(X)$ due to the smoothing of the boundary is Ch^{1-d} and we can use the bracketing of X as well.

We can even improve the remainder estimate to $o(h^{1-d})$ under the standard non-periodicity condition.

Furthermore, if the metric and potential are not smooth, we need to mollify them, taking the mollification parameter ε larger near ∂X and taking $\rho = Ch|\log h|/\varepsilon$, but it works. For systems, we can exploit the fact that most of the cones of dependence are actually trajectories. For exact statements, proofs and details, see Section 7.5 of [Ivr4].

Aftermath

After the non-smooth local theory is developed, we can use all the arguments of Section 3 and consider "stronger but more concentrated" singularities added on the top of the weaker ones.

2 Magnetic Schrödinger Operator

Introduction

This Section is entirely devoted to the study of the *magnetic Schrödinger operator*

$$H = (-ih\nabla - \mu A(x))^2 + V(x) \tag{2.1}$$

and of the Schrödinger-Pauli operator

$$H = ((-ih\nabla - \mu A(x)) \cdot \boldsymbol{\sigma})^2 + V(x) \tag{2.2}$$

with a small semiclassical parameter h and large *magnetic intensity parameter* (coupling constant) responsible for the interaction of a particle with the magnetic field μ. Here, $\boldsymbol{\sigma} = (\sigma_1, \dots, \sigma_d)$ where $\sigma_1, \dots, \sigma_d$ are Pauli $\mathsf{D} \times \mathsf{D}$-matrices and A is *magnetic vector potential*. We are interested in the two-parameter asymptotics (with respect to h and μ) as well as related asymptotics.

Standard Theory

Preliminaries

For a detailed exposition, generalizations and proofs, see Chapter 13 of [Ivr4].

Consider the most interesting cases $d = 2, 3$ with smooth $V(x)$ and $A(x)$. If $d = 2$, the magnetic field could be described by a single (pseudo)scalar $F_{12} = \partial_1 A_2 - \partial_2 A_1$ and by a scalar $F = |F_{12}|$. If $d = 3$, the magnetic field could be described by a (pseudo)vector $\boldsymbol{F} = \nabla \times A$ (*vector magnetic intensity*) and by a scalar $F = |\boldsymbol{F}|$ (*scalar magnetic intensity*). As a toy-model, we consider an operator in $\mathbb{R}^d$ with constant V and $\boldsymbol{F}$. Then canonical form of the operator (2.1) is

$$H = h^2 D_1^2 + (hD_2 - \mu F x_1)^2 + \underbracket{h^2 D_3^2} + V, \tag{2.3}$$

with the third term omitted when $d = 3$. Then we can calculate

$$e(x, x, \tau) = h^{-d} \mathcal{N}_d^{\mathsf{MW}}(\tau - V, \mu h F) \tag{2.4}$$

with

$$\mathcal{N}_d^{\mathsf{MW}}(\tau, F) = \kappa_d \sum_{n \geq 0} \bigl(\tau - (2n+1)F\bigr)_+^{\frac{1}{2}(d-2)} F, \tag{2.5}$$

where $\kappa_2 = 1/(2\pi)$, $\kappa_3 = 1/(2\pi^2)$. In particular, if $d = 2$, $F \neq 0$ this operator has a pure point spectrum of infinite multiplicity. Eigenvalues $(2m+1)\mu h F$ are called *Landau levels*. If $d = 3$, this operator has an absolutely continuous spectrum.

In these cases, the operator (2.2) is a direct sum of $\mathsf{D}/2$ operators H_- and $\mathsf{D}/2$ operators H_+ where $H_\mp = H_0 \mp \mu h F$, H_0 is the operator (2.1); then

$$\mathcal{N}_d^{\mathsf{MW}}(\tau - V, \mu h F) := \kappa_d \mathsf{D} \Bigl(\frac{1}{2} \tau_+^{\frac{1}{2}(d-2)} + \sum_{n \geq 1} \bigl(\tau - 2nF\bigr)_+^{\frac{1}{2}(d-2)}\Bigr) F \tag{2.6}$$

Classical dynamics are different as well: when $d = 2$, the trajectories are *magnetrons*–circles of radii $(\mu F)^{-1}$, while if $d = 3$, there is also free movement along *magnetic lines*–integral curves of $\boldsymbol{F}$, so the trajectories are solenoids.

Canonical Form

Using the $\hbar$-Fourier transform, we can reduce the magnetic Schrödinger operator to its microlocal canonical form

$$\mu^2 \sum_{n\geq 0} B_n(x_1, \hbar D_1, \mu^{-2}, \hbar)\mathcal{L}_0^n \qquad \text{for} \quad d=2, \tag{2.7}$$

$$h^2 D_2^2 + \mu^2 \sum_{n\geq 0} B_n(x', \hbar D_1, \mu^{-2}, \hbar)\mathcal{L}_0^n \qquad \text{for} \quad d=3, \tag{2.8}$$

with $\hbar = \mu^{-1}h$, $\mathcal{L}_0 = x_d^2 + \hbar^2 D_d^2$, $x' = x_1$ and $x' = (x_1, x_2)$ when $d = 2, 3$ respectively. Further, the principal symbols of the operators B_0 and B_1 are $\mu^{-2}V \circ \Psi$ and $F \circ \Psi$ respectively, where Ψ is a diffeomorphism $(x', \xi_1) \to x$.

This canonical form allows us to study both the classical trajectories and the propagation of singularities in the general case. When $d = 2$, there is still movement along the magnetrons but magnetrons are drifting with the velocity $\boldsymbol{v} = \mu^{-1}(\nabla((V - \tau)/F_{12}))^{\perp}$ where $^{\perp}$ denotes the counter-clockwise rotation by $\pi/2$. If $d = 3$, trajectories are solenoids winding around magnetic lines and the movement along magnetic lines is described by an 1-dimensional Hamiltonian but there there is also side-drift as in $d = 2$.

We can replace then $\mathcal{L}_0$ by its eigenvalues which are $(2j+1)\hbar$, thus arriving to a family of $\hbar$-pseudodifferential operators with respect to x_1 if $d = 2$ and to a family of $\hbar$-pseudodifferential operators with respect to x_1 which is also a Schrödinger operator with respect to x_2.

Asymptotics: Moderate Magnetic Field

We can always recover the estimate $O(\mu h^{1-d})$ with the standard Weyl principal part simply by using the scaling $x \to \mu x$, $h \mapsto \mu h$, $\mu \mapsto 1$. On the other hand, for $d = 2$, we cannot in general improve it as follows from the example with constant F and V.

However, under a(THE?) non-degeneracy assumption, the remainder estimate is much better:

Theorem 2.1. *Let* $d = 2$, $F \asymp 1$, $\mu h \lesssim 1$ *and*

$$|\nabla V F^{-1}| + |\det \operatorname{Hess} V F^{-1}| \geq \epsilon. \tag{2.9}$$

Then

$$\int \Bigl(e(x, x, 0) - h^{-2}\mathcal{N}_2^{\mathsf{MW}}(x, -V, \mu h F) \Bigr) \psi(x)\, dx = O(\mu^{-1}h^{-1}). \tag{2.10}$$

The explanation is simple: each of the non-degenerate 1-dimensional $\hbar$-pseudodifferential operators contributes $O(1)$ to the remainder estimate and there is $\asymp (\mu h)^{-1}$ of them which should be taken into account. Another explanation is that under the non-degeneracy assumption, the drift of the magnetrons destroys the periodicity but we can follow the evolution for time $T^* = \epsilon\mu$, so the remainder estimate is $O(T^{*\,-1}h^{-1})$.

If $d = 3$, we cannot get the local remainder estimate better than $O(h^{-2})$ without global non-periodicity conditions due to the evolution along magnetic lines. On the other hand, we do not need strong non-degeneracy assumptions:

Theorem 2.2. *Let $d = 3$, $F \asymp 1$ and $\mu h \lesssim 1$. Then,*

$$\int \Big(e(x, x, 0) - h^{-3}\mathcal{N}_3^{\mathsf{MW}}(x, -V, \mu hF)\Big)\psi(x)\,dx = O(h^{-2} + \mu h^{-1-\delta}) \tag{2.11}$$

in the general case and

$$\int \Big(e(x, x, 0) - h^{-3}\mathcal{N}_3^{\mathsf{MW}}(x, -V, \mu hF)\Big)\psi(x)\,dx = O(h^{-2}), \tag{2.12}$$

provided

$$\sum_{\alpha:\,1\le|\alpha|\le K} |\nabla^\alpha VF^{-1}| \ge \epsilon. \tag{2.13}$$

Further, in the general case, as(FOR?) $\mu \le h^{-\frac{1}{3}}$, we can replace the magnetic Weyl expression $\mathcal{N}_3^{\mathsf{MW}}$ by the standard Weyl expression $\mathcal{N}_3$.

Asymptotics: Strong Magnetic Field

Let us now consider the strong magnetic field case $\mu h \gtrsim 1$. Then the remainder estimates (2.10), (2.11) and (2.12) acquire a factor of μh^{-1}:

Theorem 2.3. *Let $d = 2$, $F \asymp 1$ and $\mu h \gtrsim 1$. Then for the operator* (2.3)*,*

(i) Under the assumption

$$|\tau V - (2j + 1)\mu hF| \ge \epsilon_0 \qquad \forall j \in \mathbb{Z}^+, \tag{2.14}$$

the following asymptotics holds:

$$e(x, x, \tau) - h^{-2}\mathcal{N}_2^{\mathsf{MW}}(x, \tau - V, F) = O(\mu^{-s}h^s). \tag{2.15}$$

(ii) Under the assumption

$$|\tau V-(2j+1)\mu hF|+|\nabla((V-\tau)F^{-1})|+ |\det\mathsf{Hess}((V-\tau)F^{-1})|\geq\epsilon_0 \qquad \forall j\in\mathbb{Z}^+, \tag{2.16}$$

the following asymptotics holds:

$$\int\Bigl(e(x,x,\tau)-h^{-2}\mathcal{N}_2^{\mathsf{MW}}(x,\tau-V,F)\Bigr)\psi(x)\,dx=O(1). \tag{2.17}$$

Remark 2.4. If $d=2$, we only need that $\mu^{-1}h\ll 1$ rather than $h\ll 1$.

Theorem 2.5. *Let $d=3$, $F\asymp 1$ and $\mu h\gtrsim 1$. Then for the operator* (2.3),

$$\int\Bigl(e(x,x,0)-h^{-3}\mathcal{N}_3^{\mathsf{MW}}(x,-V,\mu hF)\Bigr)\psi(x)\,dx=O(\mu h^{-1-\delta}) \tag{2.18}$$

in the general case and

$$\int\Bigl(e(x,x,0)-h^{-3}\mathcal{N}_3^{\mathsf{MW}}(x,-V,\mu hF)\Bigr)\psi(x)\,dx=O(\mu h^{-1}) \tag{2.19}$$

under the assumption

$$|V+(2j+1)\mu hF|+\sum_{\alpha\colon 1\leq|\alpha|\leq K}|\nabla^\alpha VF^{-1}|\geq\epsilon \qquad \forall j\in\mathbb{Z}^+. \tag{2.20}$$

Remark 2.6. (i) $\mathcal{N}_d^{\mathsf{MW}}=O(\mu h)$ for $\mu h\gtrsim 1$.

(ii) For the Schrödinger-Pauli operator (2.4), one only needs to replace "$(2j+1)$" by "$2j$" in the assumptions above.

2D case, Degenerating Magnetic Field

Preliminaries

Since μF plays such a prominent role when $d=2$, one may ask what happens if F vanishes somewhere? Obviously, one needs to make certain assumptions; it turns out that in the generic case

$$|F|+|\nabla F|\asymp 1, \tag{2.21}$$

the *degeneration manifold* $\Sigma := \{x :\ F(x) = 0\}$ is a smooth manifold and the operator is modelled by

$$h^2D_1^2 + (hD_2 - \mu x_1^2/2)^2 + V(x_2), \tag{2.22}$$

which we are going to study. We consider the local spectral asymptotics for ψ supported in a small enough vicinity of Σ. Under the assumption (2.21) (or, rather more a general one), the complete analysis was done in Chapter 14 of [Ivr4].

Moderate and Strong Magnetic Field

We start from the case $\mu h \lesssim 1$. Without any loss of the generality, one can assume that $\Sigma = \{x : x_1 = 0\}$. Then, the scaling $x \mapsto x/\gamma(\bar{x})$ (with $\gamma(x) = \frac{1}{2}\mathsf{dist}(x,\Sigma)$), brings us to the case of the non-degenerate magnetic field with $h \mapsto h_1 = h/\gamma$ and $\mu \mapsto \mu_1 = \mu\gamma^2$ as long as $\gamma \ge \mu^{-\frac{1}{2}}$. Then the contribution of $B(x,\gamma(x))$ to the remainder does not exceed $C\mu_1^{-1}h_1^{-1} = C\mu^{-1}h^{-1}\gamma^{-1}$ and the total contribution of the *regular zone* $\mathcal{Z} = \{\gamma(x) \ge C_0\mu^{-\frac{1}{2}}\}$ does not exceed $C\int \mu^{-1}h^{-1}\gamma^{-3}\,dx = Ch^{-1}$.

On the other hand, in the *degeneration zone* $\mathcal{Z}_0 = \{\gamma(x) \le C_0\mu^{-\frac{1}{2}}\}$, we use $\gamma = \mu^{-\frac{1}{2}}$ and the contribution of $B(x,\gamma(x))$ does not exceed $Ch_1^{-1} = Ch^{-1}\mu^{-\frac{1}{2}}$ and the total contribution of this zone also does not exceed Ch^{-1}.

Thus we conclude that the left-hand expression of (2.10) is now $O(h^{-1})$. Can we do any better than this?

Analysis of the evolution and propagation in the zone $\mathcal{Z}$ shows that there is a drift of magnetic lines along Σ with speed $C\mu^{-1}\gamma^{-1}$ which allows us to improve $T^* \asymp \mu\gamma^2$ to $T^* \asymp \mu\gamma$ (both before rescaling) and improve the estimate of the contribution of $B(x,\gamma(x))$ to $C\mu^{-1}h^{-1}$ and the total contribution of this zone to $C\int \mu^{-1}h^{-1}\gamma^{-2}\,dx = C\mu^{-\frac{1}{2}}h^{-1}$.

Analysis of evolution and propagation in the zone $\mathcal{Z}_0$ is more tricky. It turns out that there are *short periodic trajectories* with period $\asymp \mu^{-\frac{1}{2}}$, but there are not many of them which allows us to improve the remainder estimate in this zone as well.

Theorem 2.7. *Let $d = 2$ and suppose the condition* (2.21) *is fulfilled. Let $\Sigma := \{F = 0\} = \{x_1 = 0\}$ and $-V \asymp 1$. Let $\mu \le h^{-1}$. Then,*

(i) The left-hand expression of (2.17) *is $O(\mu^{-\frac{1}{2}}h^{-1} + h^{-1}(\mu^{\frac{1}{2}}h|\log h|)^{\frac{1}{2}})$. In particular, for $\mu \lesssim (h|\log h|)^{-\frac{2}{3}}$, it is $O(\mu^{-\frac{1}{2}}h^{-1})$.*

(ii) Further,

$$\int \Bigl(e(x,x,0) - h^{-2}\mathcal{N}_2^{\mathsf{MW}}(x,-V,\mu hF)\Bigr)\psi(x)\,dx - h^{-1}\int \mathcal{N}^{\mathsf{MW}}_{\mathsf{corr}}(x_2,0)\psi(x_2,0) = O(\mu^{-\frac{1}{2}}h^{-1}+h^{-\delta}) \tag{2.23}$$

with

$$h^{-1}\mathcal{N}^{\mathsf{MW}}_{\mathsf{corr}} := (2\pi h)^{-1}\int \boldsymbol{n}_0(\xi_2,-W(x_2),\hbar)\,d\xi_2 - h^{-2}\int \mathcal{N}^{\mathsf{MW}}(-W(x_2),\mu hF(x_1))\,dx_1 \tag{2.24}$$

where $\boldsymbol{n}_0(\xi_2,\tau,\hbar)$ *is an eigenvalue counting function for the operator* $\boldsymbol{a}_0(\xi_2,\hbar) = \hbar^2 D_1^2 + (\xi_2 - x_1^2/2)^2$ *on* $\mathbb{R}^1 \ni x_1$, $\hbar = \mu^{\frac{1}{2}}h$ *and* $W(x_2) = V(0,x_2)$.

(iii) Furthermore, under the non-degeneracy assumption

$$\sum_{1\le k\le m} |\partial_{x_2}^k W| \asymp 1 \tag{2.25}$$

(in the framework of assumption (2.22)*), one can take* $\delta = 0$ *in* (2.23).

Remark 2.8. (i) Under some non-degeneracy assumptions, Theorem 2.7(i) could also be improved.

(ii) Theorem 2.7 remains valid for $h^{-1} \le \mu \lesssim h^{-2}$ as well but then the zone $\{x:\ \gamma(x) \ge C(\mu h)^{-1}\}$ is forbidden, contribution to the principal part is delivered by the zone $\{x:\ \gamma(x) \lesssim (\mu h)^{-1}\}$ and it is $\lesssim \mu^{-1}h^{-3}$.

(iii) As $\mu \ge Ch^2$, the principal part is 0 and the remainder is $O(\mu^{-s})$.

For further details, generalizations and proofs, see Section 14.6 of [Ivr4].

Strong and Superstrong Magnetic Field

Assume now that $\mu \gtrsim h^{-1}$ and replace V by $V - (2j+1)\mu h F_{12}$ with $j \in \mathbb{Z}^+$. Then the zone $\{x:\ \gamma(x) \ge C(\mu h)^{-1}\}$ is no longer forbidden, the principal part of asymptotics is of the magnitude μh^{-1} (cf. Remark 2.8(ii) and the remainder estimate becomes $O(\mu^{-\frac{1}{2}}h^{-1} + h^{-\delta})$ (and under the non-degeneracy assumption one can take $\delta = 0$).

Furthermore, the case $\mu \geq Ch^{-2}$ is no longer trivial. First, one needs to change the correction term by replacing $\boldsymbol{a}_0$ with $\boldsymbol{a}_{2j+1} := \boldsymbol{a}_0 - (2j+1)\hbar x_1$. Second, the non-degeneracy condition should be relaxed by requiring (2.25) only if

$$|\hbar^{2/3}\lambda_{j,n}(\eta) + W(x_2)| + |\partial_\eta \lambda_{j,n}(\eta) \geq \epsilon \qquad \forall \eta, \tag{2.26}$$

fails, where $\lambda_{j,n}$ are the eigenvalues of $\boldsymbol{a}_{2j+1}$ with $\hbar = 1$.

Furthermore, if

$$|\hbar^{2/3}\lambda_{j,n}(\eta) + W(x_2)| \geq \epsilon \qquad \forall \eta, \tag{2.27}$$

then 0 belongs to the spectral gap and the remainder estimate is $O(\mu^{-s})$.

For further details, exact statements, generalizations and proofs, see Sections 14.7 and 14.8 of [Ivr4].

2D Case, near the Boundary

Moderate Magnetic Field

We now consider the magnetic Schrödinger operator with $d = 2$, $F \asymp 1$ in a compact domain X with $\mathscr{C}^\infty$-boundary. While the dynamics inside the domain do not change, the dynamics in the boundary layer of the width $\asymp \mu^{-1}$ are completely different. When the magnetron hits ∂X, it reflects according to the standard "incidence angle equals reflection angle" law and thus the "particle" propagates along ∂X with speed $O(1)$ rather than $O(\mu^{-1})$. Therefore, physicists distinguish between *bulk* and *edge particles*. Note however that in general, this distinction is not as simple as in the case of constant F and V. Indeed, a drifting inner trajectory can hit ∂X and become a *hop trajectory*, while the latter could leave the boundary and become an inner trajectory.

It follows from Section 2 that the contribution of $B(x, \gamma(x))$ with $\gamma(x) = \frac{1}{2}\mathsf{dist}(x, \partial X) \geq \bar\gamma = C\mu^{-1}$ to the remainder is $O(\mu^{-1}h^{-1}\gamma^2 T(x)^{-1})$, where $T(x)$ is the length of the drift trajectory inside the *bulk zone* $\{x \in X : \gamma(x) \geq \bar\gamma\}$. Then the total contribution of this zone to the remainder does not exceed $C\mu^{-1}h^{-1}\int T(x)^{-1}\,dx = O(\mu^{-1}h^{-1})$ since $T(x) \gtrsim \gamma(x)^{\frac{1}{2}}$ (in the proper direction).

On the other hand, due to the rescaling $x \mapsto x/\bar\gamma$, the contribution of $B(x, \bar\gamma)$ with $\gamma(x) \leq \bar\gamma$ to the remainder does not exceed $C\mu h^{-1}\bar\gamma^2$ and the total contribution of the *edge zone* $\{x \in X : \gamma(x) \le \bar{\gamma}\}$ does not exceed $C\mu h^{-1}\bar{\gamma} = Ch^{-1}$ and the total remainder is $O(h^{-1})$. Thus, if we want a better estimate, we need to study propagation along ∂X.

Theorem 2.9. *Under the non-degeneracy assumption* $|\nabla_{\partial X}(VF^{-1})| \asymp 1$ *on* $\mathsf{supp}(\psi)$ *(contained in the small vicinity of* ∂X*) for* $\mu h \lesssim 1$

$$\int_X \Bigl(e(x,x,0) - h^{-2}\mathcal{N}^{\mathsf{MW}}(x,0,\mu h)\Bigr)\psi(x)\,dx - h^{-1}\int_{\partial X} \mathcal{N}^{\mathsf{MW}}_{*,\mathsf{bound}}(x,0,\mu h)\psi(x)\,ds_g = O(\mu^{-1}h^{-1}), \tag{2.28}$$

where $\mathcal{N}^{\mathsf{MW}}_{*,\mathsf{bound}}$ *is introduced in* $(5.4.2)_{\mathsf{D}}$ *or* $(5.4.2)_{\mathsf{N}}$ *below for the Dirichlet or Neumann boundary conditions respectively with* $\hbar = \mu h F(x)$ *and* τ *replaced by* $-V(x)$.

Here,

$(5.4.2)_{\mathsf{D}}$ $\mathcal{N}^{\mathsf{MW}}_{\mathsf{D},\mathsf{bound}}(\tau,\hbar) :=$

$$(2\pi)^{-1}\int_0^\infty \sum_{j\ge 0}\Bigl(\int \theta\bigl(\tau - \hbar\lambda_{\mathsf{D},j}(\eta)\bigr)\upsilon^2_{\mathsf{D},j}(x_1,\eta)\,d\eta - \theta\bigl(\tau-(2j+1)\hbar\bigr)\Bigr)\hbar^{\frac{1}{2}}\,dx_1$$

and

$(5.4.2)_{\mathsf{N}}$ $\mathcal{N}^{\mathsf{MW}}_{\mathsf{N},\mathsf{bound}}(\tau,\hbar) :=$

$$(2\pi)^{-1}\int_0^\infty \sum_{j\ge 0}\Bigl(\int \theta\bigl(\tau - \hbar\lambda_{\mathsf{N},j}(\eta)\bigr)\upsilon^2_{\mathsf{N},j}(x_1,\eta)\,d\eta - \theta\bigl(\tau-(2j+1)\hbar+\bigr)\Bigr)\hbar^{\frac{1}{2}}\,dx_1,$$

where $\lambda_{\mathsf{D},j}(\eta)$ *and* $\lambda_{\mathsf{N},j}(\eta)$ *are eigenvalues and* $\upsilon_{\mathsf{D},j}$ *and* $\upsilon_{\mathsf{N},j}$ *are eigenfunctions of operator*

$$a(\eta,x_1,D_1) = D_1^2 + x_1^2 \qquad \text{as}\quad x_1 < \eta \tag{2.30}$$

with the Dirichlet or Neumann boundary conditions respectively at $x_1 = \eta$.

Remark 2.10. Under weaker non-degeneracy assumptions $|\nabla VF^{-1}| \asymp 1$ and $\nabla_{\partial X} VF^{-1} = 0 \implies \pm\nabla^2_{\partial X} VF^{-1} \ge \epsilon$, less sharp remainder estimates are derived. The sign in the latter inequality matters since it affects the dynamics. It also matters whether Dirichlet or Neumann boundary conditions are considered: for the Dirichlet boundary condition we get a better remainder estimate.

For exact statements, generalizations and proofs, see Sections 15.2 and 15.2 of [Ivr4].

Strong Magnetic Field

We now consider the strong magnetic field $\mu h \gtrsim 1$ and for simplicity assume that $F = 1$. In this case, we need to study an auxillary operator $D_1^2 + (x_1 - \eta)^2$ as $x_1 < 0$ with either the Dirichlet or Neumann boundary conditions at $x_1 = 0$ or equivalently the operator (2.30) and our operator is basically reduced to a perturbed operator

$$a(\hbar D_2, x_1, D_1) - (2j+1) - (\mu h)^{-1} W(x_2) \qquad \hbar = \mu^{-1} h, \tag{2.31}$$

with $W(x_2) = V(0, x_2)$. Then we need to analyze either $\lambda_{\mathsf{D},j}(\eta)$ or $\lambda_{\mathsf{N},j}(\eta)$ more carefully. It turns out that:

Proposition 2.11. *$\lambda_{\mathsf{D},n}(\eta)$ and $\lambda_{\mathsf{N},n}(\eta)$, $n = 0, 1, 2, ...$ are real analytic functions with the following properties:*

(i) $\lambda_{\mathsf{D},k}(\eta)$ are monotone decreasing for $\eta \in \mathbb{R}$; $\lambda_{\mathsf{D},k}(\eta) \nearrow +\infty$ as $\eta \to -\infty$; $\lambda_{\mathsf{D},k}(\eta) \searrow (2k+1)$ as $\eta \to +\infty$; $\lambda_{\mathsf{D},k}(0) = (4k+3)$.

(ii) $\lambda_{\mathsf{N},k}(\eta)$ are monotone decreasing for $\eta \in \mathbb{R}^-$; $\lambda_{\mathsf{N},k}(\eta) \nearrow +\infty$ as $\eta \to -\infty$; $\lambda_{\mathsf{N},k}(\eta) < (2n+1)$ as $\eta \geq (2n+1)^{\frac{1}{2}}$; $\lambda_{\mathsf{N},k}(0) = (4n+1)$.

(iii) $\lambda_{\mathsf{N},k}(\eta) < \lambda_{\mathsf{D},k}(\eta) < \lambda_{\mathsf{N},(k+1)}(\eta)$; $\lambda_{\mathsf{D},k}(\eta) > (2k+1)$, $\lambda_{\mathsf{N},n}(\eta) > (2k-1)_+$.

Proposition 2.12. *(i) $\partial_\eta \lambda_{\mathsf{D},k}(\eta) < 0$.*

(ii) $\partial_\eta \lambda_{\mathsf{N},n}(\eta) \gtreqless 0$ if and only if

$$\lambda_{\mathsf{N},k}(\eta) \lesseqgtr \eta^2. \tag{2.32}$$

(iii) $\lambda_{\mathsf{N},k}(\eta)$ has a single stationary point[38] η_k, it is a non-degenerate minimum, and at this point (2.32) *holds.*

(iv) In particular, $(\lambda_{\mathsf{N},k}(\eta) - \eta^2)$ has the same sign as $(\eta_k - \eta)$.

[38] And it must have one due to Proposition 2.11.

We see the difference between the Dirichlet and Neumann cases because we need non-degeneracy for $\lambda_{*,k}(\hbar D_2) - (2j+1) + W(x_2)$. It also means the difference in the propagation of singularities along ∂X: in the Dirichlet case, all singularities move in one direction (constant sign of $\lambda'_{\mathsf{D},k}$), while in the Neumann case, some move in the opposite direction (variable sign of $\lambda'_{\mathsf{N},k}$); this effect plays a role also in the case when $\mu h \lesssim 1$.

Assume here that τ is in an "inner" spectral gap:

$$|(2j+1)\mu h + V - \tau| \ge \epsilon_0 \mu h \qquad \forall x\ \forall j \in \mathbb{Z}^+. \tag{2.33}$$

Theorem 2.13. *Suppose that $\mu h \gtrsim 1$ and the condition* (2.33) *is fulfilled. Then,*

(i) In case of the Dirichlet boundary condition, the left-hand expression in (2.28) *is $O(1)$.*

(ii) In case of the Neumann boundary condition, assume additionally that

$$(5.4.7)_\pm \quad |(\lambda_{\mathsf{N},j}(\eta)\mu h + V - \tau| \le \epsilon_0 \mu h,$$
$$|\lambda'_{\mathsf{N},j}(\eta)| + |\partial_{x_2} V| \le \epsilon_0 \implies \pm \partial^2_{x_2} V \ge \epsilon_0 \qquad \forall j = 0, 1, 2, ...$$

Then, the left-hand expression in (2.28) *is $O(1)$ under the assumption* $(2.34)_+$ *and $O(\log h)$ under the assumption* $(2.34)_-$.

Remark 2.14. (i) If (2.33) is fulfilled for all $\tau \in [\tau_1, \tau_2]$, then the asymptotics is "concentrated" in the boundary layer.

(ii) For a more general statement when (2.33) fails (i.e. when τ is no longer in the "inner" spectral gap) and is replaced with the condition

$$|V + (2j+1)\mu h - \tau| + |\nabla V| \asymp 1 \tag{2.35}$$

on $\mathsf{supp}(\psi)$, see Theorem 15.4.18 of [Ivr4].

Pointwise Asymptotics and Short Loops

We are now interested in the pointwise asymptotics inside the domain. Surprisingly, it turns out that the standard Weyl formula for this purpose is better than the Magnetic Weyl formula.

Case $d=2$

We start from the case $d=2$, $F=1$, $|\nabla V|\asymp 1$. One can easily see that in classical dynamics, short loops of the lengths $\asymp \mu^{-1}n$ with $n=1,\dots,N$, $N\asymp\mu$ appear. We would like to understand how these loops affect the asymptotics in question.

Theorem 2.15. *For the magnetic Schrödinger operator which satisfies the above assumptions in a domain $X\subset\mathbb{R}^2$, with $B(0,1)\subset X$, the following estimates hold at a point $x\in B(0,\frac{1}{2})$*

(i) For $1\le\mu\le h^{-\frac{1}{2}}$,

$$|e(x,x,\tau)-h^{-2}\mathcal{N}_x^{\mathsf{W}}(\tau)|\le C\mu^{-1}h^{-1}+C\mu^{\frac{1}{2}}h^{-\frac{1}{2}}+C\mu^2h^{-\frac{1}{2}} \tag{2.36}$$

and

$$\begin{aligned}\mathsf{R}^{\mathsf{W}}_{x(r)}\coloneqq |e(x,x,0)-h^{-2}\bigl(\mathcal{N}^{\mathsf{W}}_x(0)+\mathcal{N}^{\mathsf{W}}_{x,\mathsf{corr}(r)}(0)\bigr)|\le\\ C\mu^{-1}h^{-1}+C\mu^{\frac{1}{2}}h^{-\frac{1}{2}}+C\mu h^{-1}\bigl(\mu^2h\bigr)^{r+\frac{1}{2}}+\\ C\begin{cases}\Bigl(h^{-1}\bigl(h\mu^{\frac{5}{2}}\bigr)^{r+\frac{1}{2}}+\mu^{\frac{1}{3}}h^{-\frac{2}{3}}\Bigr) & \text{as}\quad \mu\le h^{-\frac{2}{5}},\\ \mu^{\frac{5}{3}}h^{-\frac{1}{3}} & \text{as}\quad \mu\ge h^{-\frac{2}{5}}\end{cases}\end{aligned} \tag{2.37}$$

where $\mathcal{N}^{\mathsf{W}}_{x,\mathsf{corr}(r)}$ is the r-term stationary phase approximation to some explicit oscillatory integral (see Section 16.3 of [Ivr4]).

(ii) For $h^{-\frac{1}{3}}\le\mu\le h^{-1}$,

$$\begin{aligned}\mathsf{R}^{\mathsf{W}\prime\prime}_{x(r)}\coloneqq\\ |\Bigl(e(x,x,\tau)-h^{-2}\mathcal{N}_{x,\mathsf{corr}(r)}-\bar{e}_x(x,x,\tau)+h^{-2}\bar{\mathcal{N}}_{x,\mathsf{corr}(r)}\Bigr)|\le\\ C\mu^{\frac{1}{2}}h^{-\frac{1}{2}}+C\begin{cases}\mu^{-2}h^{-2}(\mu^2h)^{r+\frac{1}{2}} & \text{for}\quad \mu\le h^{-\frac{1}{2}}\\ h^{-1} & \text{for}\quad \mu\ge h^{-\frac{1}{2}}\end{cases}\\ +C\begin{cases}h^{-1}\bigl(\mu^{\frac{5}{2}}h\bigr)^{r+\frac{1}{2}}+\mu^{\frac{1}{3}}h^{-\frac{2}{3}} & \text{for}\quad \mu\le h^{-\frac{2}{5}}\\ \mu^{\frac{5}{3}}h^{-\frac{1}{3}} & \text{for}\quad h^{-\frac{2}{5}}\le\mu\le h^{-\frac{1}{2}}\\ \mu^{-\frac{1}{3}}h^{-\frac{4}{3}} & \text{as}\quad \mu\ge h^{-\frac{1}{2}}\end{cases}\end{aligned} \tag{2.38}$$

while for $r = 0$,

$$\mathsf{R}^{\mathsf{W}\prime\prime}_{x(0)} := |e(x,x,\tau) - \bar{e}_x(x,x,\tau)| \le C\mu^{\frac{1}{2}}h^{-\frac{1}{2}} + C\begin{cases} h^{-1}\mu^{\frac{1}{2}} & \text{for } \mu \le h^{-\frac{1}{2}}, \\ \mu^{-\frac{1}{2}}h^{-\frac{3}{2}} & \text{for } \mu \ge h^{-\frac{1}{2}} \end{cases} \tag{2.39}$$

where here and in (iii), $\bar{e}_y$ *is constructed for the toy-model in* y *(with* $F = F(y)$ *and* $V(x) = V(y) + \langle \nabla V(y), x - y\rangle$*).*

(iii) For $\mu \ge h^{-1}$, $\tau \le c\mu h$,

$$|e(x,x,\tau) - \bar{e}_x(x,x,\tau)| \le C\mu^{\frac{1}{2}}h^{-\frac{1}{2}}. \tag{2.40}$$

Case $d = 3$

For $d = 3$, we cannot expect a remainder estimate better than $O(h^{-1})$. On the other hand, the purely Weyl approximation has a better chance to succeed as the loop condition now includes returning free movement along the magnetic line in addition to the returning circular movement. We formulate only one theorem out of many from Section 16.7 of [Ivr4]:

Theorem 2.16. *Let* $d = 3$. *Then,*

(i) In the general case,

$$|e(x,x,\tau) - h^{-3}\mathcal{N}^{\mathsf{W}}_x(x,x,\tau)| \le Ch^{-2} + C\mu^{\frac{3}{2}}h^{-\frac{3}{2}}. \tag{2.41}$$

(ii) Under non-degeneracy condition

$$|\nabla_{\perp \boldsymbol{F}}(V - \tau)/F| \asymp 1, \tag{2.42}$$

where $\nabla_\perp$ *is the component of the gradient perpendicular to* $\boldsymbol{F}$, *for* $\mu \le h^{-\frac{1}{2}}$, *we have the estimates*

$$|e(x,x,\tau) - h^{-3}\mathcal{N}^{\mathsf{W}}_x(x,x,\tau)| \le Ch^{-2} + C\mu^{\frac{5}{2}}h^{-1} \tag{2.43}$$

and

$$|e(x,x,\tau) - h^{-3}\mathcal{N}^{\mathsf{W}}_x(x,x,\tau) - h^{-3}\mathcal{N}_{x,\mathsf{corr}(r)}| \le Ch^{-2} + C\mu^{\frac{3}{2}}h^{-\frac{3}{2}}(\mu^2 h)^{r+\frac{1}{2}}. \tag{2.44}$$

Here we use stationary phase approximations again.

Remark 2.17. One can also consider the cases $h^{-\frac{1}{2}} \lesssim \mu \lesssim h^{-1}$ and $\mu \gtrsim h^{-1}$. But then one needs to include the toy-model expression (with constant $\boldsymbol{F}$ and ∇V) into the approximation.

Related Asymptotics

Apart from the pointwise asymptotics, one can consider the related asymptotics of

$$\int \omega(\frac{1}{2}(x+y), x-y)e(x,y,\tau)e(y,x,\tau)\,dxdy \tag{2.45}$$

and estimates of

$$\int \omega(\frac{1}{2}(x+y), x-y)\bigl(e(x,x,\tau)-e^{\mathsf{W}}(x,x,\tau)\bigr)\times \bigl(e(y,y,\tau)-e^{\mathsf{W}}(y,y,\tau)\bigr)\,dxdy. \tag{2.46}$$

For all the details, see Chapter 16 of [Ivr4]. These expressions play important role in Section 4.

Magnetic Dirac oOperators

We discuss the magnetic Dirac operators

$$H = ((-ih\nabla - \mu A(x))\cdot \boldsymbol{\sigma}) + \sigma_0 M + V(x) \tag{2.47}$$

and

$$H = ((-ih\nabla - \mu A(x))\cdot \boldsymbol{\sigma}) + V(x). \tag{2.48}$$

If $d=3$, for the second operator, we can consider 2×2 matrices rather than 4×4 matrices.

If $V=0$ then H^2 equals to the Schrödinger-Pauli operator (plus M^2) and therefore the theory of magnetic Dirac and Schrödinger operators are closely connected. If $V=0$ and $0\ne \boldsymbol{F}$ is constant then the operator for $d=2$ has a pure point spectrum of infinite multiplicity consisting of $\pm\sqrt{M^2+2j\mu hF}$ with $j\in\mathbb{Z}^+$ [39] and for $d=3$, this operator has absolutely continuous spectrum $(-\infty,-M]\cup[M,\infty)$. Thus we get corresponding *Landau levels*.

The results similar to those of Section 2 hold (for details, exact statements and proofs, see Chapter 17 of [Ivr4]. Further, the results of Sections 2 and 2 probably are not difficult to generalize, and maybe the results of Section 2 as well under correctly posed boundary conditions.

[39] However, one of the points $\pm M$ is missing depending on whether $F_{12}\gtrless 0$ and $\sigma_1\sigma_2\sigma_3=\pm i$.

3 Magnetic Schrödinger Operator. II

Higher Dimensions

General Theory

We can consider a magnetic Schrödinger (and also Schrödinger-Pauli and Dirac) operators in higher dimensions. In this case, the magnetic intensity is characterized by the skew-symmetric matrix $F_{jk} = \partial_j A_k - \partial_k A_j$ rather than by a pseudo-scaler F_{12} or a pseudo-vector $\boldsymbol{F}$. As a result, the magnetic Weyl expression becomes more complicated; as before, it is exactly $e(x, x, \tau)$ for the operator in $\mathbb{R}^d$ if F_{jk} and V constant:

$$(3.1)\quad h^{-d}\mathcal{N}_d^{\mathsf{MW}}(\tau) := (2\pi)^{-r}\mu^r h^{-r}\sum_{\alpha\in\mathbb{Z}^{+r}}\Bigl(\tau - \sum_j (2\alpha_j+1)f_j\mu h - V\Bigr)_+^{\frac{1}{2}(d-2r)} f_1\cdots f_r\sqrt{g},$$

where $2r = \operatorname{rank}(F_{jk})$ and $\pm i f_j$ (with $j = 1, \dots, r$, $f_j > 0$) are its eigenvalues[40] which are not 0; recall that $z_+^0 = \theta(z)$.

One can see that H has pure point of infinite multiplicity spectrum when $d = 2r$ and H has an absolutely continuous spectrum when $d > 2r$. In any case, the bottom of the spectrum is $\mu h(f_1 + \dots + f_r)$.

We are interested in the asymptotics with the sharpest possible remainder estimate like the one for $d = 2$ or $d = 3$ in the cases $d = 2r$ and $d > 2r$ respectively[41]. Asymptotics without a remainder estimate were derived in [Rai1, Rai2].

As we try to reduce the operator to the canonical form, we immediately run into problem of *resonances* when $f_1 m_1 + \dots + f_r m_r = 0$ at some point with $m \in \mathbb{Z}^d$; $|m_1| + \dots + |m_r|$ is *an order of resonance*. If the lowest order of resonances is k, then we can reduce the operator to its canonical form modulo $O(\mu^{-k})$ for $\mu h \le 1$ (when $\mu h \ge 1$, this problem is less acute).

It turns out, however, that we can deal with an incomplete canonical form (with a sufficiently small remainder term).

Another problem is that we cannot in general assume that the f_j are constant (for $d = 2, 3$, we could achieve this by multiplying the operator by $f_1^{-1/2}$) and the microhyperbolicity condition becomes really complicated.

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[40] In the general case, the eigenvalues of $(F^j_k) = (g^{jl})(F_{lk})$ where (g^{jk}) is a metric.

[41] We assume that $(F_{jk}(x))$ has constant rank.

Case $2r = d$ In this case, only the resonances of orders $2, 3$ matter as we are looking for an error $O(\mu^{-1}h^{1-d})$ when $\mu h \le 1$. If the magnetic field is weak enough, we use the incomplete canonical form only to study propagation of the singularities and if the magnetic field is sufficiently strong, the omitted terms $O(\mu^{-4})$ in the canonical form are small enough to be neglected.

As a result, the indices $j = 1, \dots, r$ are broken into several groups (indices j and k belong to the same group if they "participate" in the resonance of order 2 or 3 after all the reductions). Then under a certain non-degeneracy assumption called $\mathfrak{N}$-microhyperbolicity (see Definition 19.2.5 of [Ivr4]) in which this group partition plays a role, we can recover the remainder estimate $O(\mu^{-1}h^{1-d})$ for $\mu h \lesssim 1$ (in which case, the principal part has magnitude h^{-d}) and $O(\mu^{r-1}h^{1-d+r})$ for $\mu h \gtrsim 1$ (in which case, the principal part has magnitude $\mu^r h^{r-d}$). If we ignore the resonances of order 3, we get a partition into smaller groups and we need a weaker non-degeneration assumption called microhyperbolicity (see Definition 19.2.4 of [Ivr4]) but the remainder estimate would be less sharp.

In an important special case of constant $f_1, \dots, f_r$, both these conditions are equivalent to $|\nabla V|$ disjoint from 0 (on $\mathsf{supp}(\psi)$) but it could be weakened to V having only non-degenerate critical points (if there are saddles, we need to add a logarithmic factor to the remainder estimate).

On the other hand, without any non-degeneracy assumptions, the remainder estimate can be as bad as $O(\mu h^{1-d})$ for $\mu h \lesssim 1$ and as bad as the principal part itself for $\mu h \gtrsim 1$.

For exact statements, details, proofs and generalizations, see Chapter 19 of [Ivr4].

Case $2r < d$ In this case, only the resonances of order 2 matter since we are expecting a larger error than in the previous case. As a result, the indices $j = 1, \dots, r$ are broken into several groups (indices j and k belong to the same group if $f_j = f_k$).

Then under a certain non-degeneracy assumption called microhyperbolicity (see Definition 20.1.2 of [Ivr4]) in which this group partition plays a role, we can recover the remainder estimate $O(h^{1-d})$ for $\mu h \lesssim 1$ (then the principal part is of the magnitude h^{-d}) and $O(\mu^r h^{1-d+r})$ for $\mu h \gtrsim 1$ (then the principal part is of the magnitude $\mu^r h^{r-d}$).

In an important special case of constant $f_1, \dots, f_r$, this condition is equivalent to $|\nabla V|$ being disjoint from 0 (on $\mathsf{supp}(\psi)$) but it could be weakened to "$\nabla V = 0 \implies \mathsf{Hess}\, V$ has a positive eigenvalue"; if we assume only that "$\nabla V = 0 \implies \mathsf{Hess}\, V$ has a non-zero eigenvalue", but we need to add a logarithmic factor to the remainder estimate.

As expected, for $2r = d-1$, we can recover less sharp remainder estimates even without any non-degeneracy assumptions and for $2r \le d-2$, we do not need any non-degeneracy conditions at all. For exact statements, details, proofs and generalizations, see Chapter 20 of [Ivr4].

Case $d = 4$: More Results

This case is simpler than the general one since we have only f_1 and f_2 and resonance happens if either $f_1 = f_2$ or $f_1 = 2f_2$ (or $f_2 = 2f_1$).

If we assume that the magnetic intensity matrix (F_{jk}) has constant rank 4, this case is simpler than the general one ($d = 2r$) and we can recover sharp remainder estimates under less restrictive conditions. For exact statements, details, proofs and generalizations, see Chapter 22 of [Ivr4].

On the other hand, if we consider (F_{jk}) of variable rank, then in the generic case, it has the eigenvalues $\pm i f_1$ and $\pm i f_2$ and $\Sigma = \{x :\ f_1(x) = 0\}$ is a $\mathscr{C}^\infty$ manifold of dimension 3, $\nabla f_1 \ne 0$ on Σ, while f_2 is disjoint from 0. It is similar to a 2-dimensional operator which we considered in Section 2, although with a twist: the symplectic form restricted to Σ has rank 2 everywhere except on a 1-dimensional submanifold Λ where it has rank 0.

Our results are also similar to those of Section 2 with rather obvious modifications but the proofs are more complicated.

For exact statements, details, proofs and generalizations, see Chapter 21 of [Ivr4].

Non-Smooth Theory

As in Chapter 4, we do not need to assume that the coefficients are very smooth. As before, we bracket the operator in question between two "rough" operators with the same asymptotics and with sharp remainder estimates. However, the lack of sufficient smoothness affects the reduction to the canonical form: it will be incomplete even if there are no resonances. Because of this, to get as sharp asymptotics as in the smooth case, we need to request more smoothness than in Chapter 4.

Case $d = 2$ For $d = 2$, we require smoothness of F_{12}, g^{jk} and V marginally larger than $\mathscr{C}^2$ to recover the same remainder estimate as in the smooth case, but there is a twist: unless the smoothness is $\mathscr{C}^3$, a correction term needs to be included. This is due to the fact that $V(x)$ and $W(x)$ differ and a more precise formula should use $W(x)$ rather than $V(x)$. Here, W is V averaged along a magnetron with center x. In fact, it is possible to consider V of the lesser smoothness than $\mathscr{C}^2$ (but marginally better than $\mathscr{C}^1$), but one gets a worse remainder estimate. For exact statements, details and proofs, see Chapter 18 of [Ivr4] and especially Section 18.5.

Case $d = 3$ Results are similar to those in the smooth case. However, in this case, if we assume no non-degeneracy conditions then the exponent δ in the estimates (2.11) and (2.18) depends on the smoothness and if we assume a non-degeneracy condition (2.13) or (2.20) then obviously K depends on the smoothness. Under the non-degeneracy assumption with $K = 1$, we need smoothness marginally better than $\mathscr{C}^1$ but again unless the smoothness is $\mathscr{C}^2$, we need to use the averaged potential $W(x)$ rather than $V(x)$.

For exact statements, details and proofs, see Chapter 18 of [Ivr4] and especially Section 18.9.

Case $d \geq 4$ Basically, the results are similar to those for $d = 2$ (if $\mathsf{rank}(F_{jk}) = d$) or for $d = 3$ (if $\mathsf{rank}(F_{jk}) < d$), but we cannot recover the sharp remainder estimate if the smoothness of V is less than $\mathscr{C}^3$ or $\mathscr{C}^2$ respectively because we cannot replace $V(x)$ by its average $W(x)$ in the canonical form.

For exact statements, details and proofs, see Chapters 19 (if $\mathsf{rank}(F_{jk}) = d$) and Chapters 20 (if $\mathsf{rank}(F_{jk}) < d$) of [Ivr4].

Global Asymptotics

For magnetic Schrödinger and Dirac operators, one can derive results similar to those of Sections 3 and 3. We describe here only some results which are very different from those already mentioned and only for the Schrödinger operator.

Case $d = 2r$

Assume that $F_{jk} = \mathsf{const}$, $\mathsf{rank}(F_{jk}) = 2r = d$, $\mu = h = 1$ and V decays at infinity. Then instead of an eigenvalue of infinite multiplicity $\lambda_{j,\infty} = (2j_1+1)f_1 + \dots + (2j_r+1)f_r$ (with $j \in \mathbb{Z}^{+\,r}$), we have a sequence of eigenvalues $\lambda_{j,n}$ tending to $\lambda_{j,\infty}$ as $n \to \infty$ and we want to consider the asymptotics of $\mathsf{N}_j^-(\eta)$ which is the number of eigenvalues in $(\lambda_{j,\infty} - \epsilon, \lambda_{j,\infty} - \eta)$ and $\mathsf{N}_j^+(\eta)$ which is the number of eigenvalues in $(\lambda_{j,\infty} + \eta, \lambda_{j,\infty} + \epsilon)$, as $\eta \to +0$.

It turns out that in contrast to the Schrödinger operator without a magnetic field, there are meaningful results no matter how fast V decays.

Theorem 3.1. *Let us consider a Schrödinger operator in $\mathbb{R}^2$ satisfying the above conditions, $\mu = h = 1$ and*

$$|\nabla^\alpha V| \le c_\alpha \rho^2 \gamma^{-|\alpha|}, \tag{3.2}$$

with $\rho = \langle x\rangle^m$, $\gamma = \langle x\rangle$, $m < 0$. Let

$$\mp V \ge -\epsilon\rho^2 \implies |\nabla V| \ge \epsilon\rho^2\gamma^{-1} \qquad \text{for } |x| \ge c. \tag{6.3.2$_\mp$}$$

Then,

(i) The asymptotics

$$\mathsf{N}_j^\mp(\eta) = \mathcal{N}^\mp(\eta) + O(\log\eta) \tag{6.3.3$_\pm$}$$

hold with

$$\mathcal{N}^\mp(\eta) = \frac{1}{2\pi}\int_{\{\mp V > \eta\}} F\,dx \tag{6.3.4$_\pm$}$$

and in our conditions $\mathcal{N}^\mp(\eta) = O(\eta^{1/m})$. Moreover, $\mathcal{N}^\mp(\eta) \asymp \eta^{1/m}$ provided that $\mp V \ge \epsilon\rho^2$ for $x \in \Gamma$, where Γ is a non-empty open sector (cone) in $\mathbb{R}^2$.

(ii) Furthermore, if

$$\mp V \ge \epsilon\rho^2 \qquad \text{for } |x| \ge c, \tag{6.3.5$_\pm$}$$

then the remainder estimate is $O(1)$. In this case, the points $(2j+1)F \pm 0$ are not limit points of the discrete spectrum.

This theorem is proved by rescaling the results of Subsection 2 which do not require $h \ll 1$, but only $\mu h \gtrsim 1$ and $\mu^{-1}h \ll 1$ (see Remark 2.4); in our case, after rescaling $\mu = 1/\rho\gamma$ and $\mu = \gamma/\rho$, so that $\mu h = 1/\rho^2$ and $\mu^{-1}h = \gamma^{-2}$. Therefore, the remainder does not exceed $\int \gamma^{-2}\,dx$, where we integrate over $\{x : |V(x)| \ge (1-\epsilon)\eta\}$ in the general case and over $\{x : (1+\epsilon)\eta \ge |V(x)| \ge (1-\epsilon)\eta\}$ under the assumption (6.3.5)$_\pm$.

Remark 3.2. (i) Similar results hold in the d-dimensional case ($d \geq 4$) when $(F) = \mathsf{const}$ and $d = \mathsf{rank}(F)$: the remainder is $O(\eta^{(d-2)/2m})$ and the principal part is $O(\eta^{d/2m})$.

(ii) One can consider the case $\rho = \exp(-\langle x\rangle^m)$, $\gamma = \langle x\rangle^{1-m}$, $0 < m < 1$, and recover remainder estimate $O(|\log\eta|^{(d-2)/m+2})$ in the general case and $O(|\log\eta|^{(d-2)/m+1})$ under the assumption (6.3.5)$_\pm$ with $\mathcal{N}^{\mp}(\eta) = O(|\log\eta|^{d/m})$.

(iii) On the other hand, the cases when V decays like $\exp(-2\langle x\rangle)$ or faster, or is compactly supported, are out of reach of our methods but the asymptotics (without a remainder estimate) were obtained in [MR, RT, RW].

For exact statements, details, proofs and generalizations for arbitrary $\mathsf{rank}(F_{jk}) = d = 2r$, see Subsection 23.4.1 of [Ivr4].

Case $d > 2r$. I

This case is less “strange” than case $d = 2$. Here, we can discuss only the eigenvalue counting function $\mathsf{N}_0^-(\eta)$.

Theorem 3.3. *Let us consider a Schrödinger operator in* $\mathbb{R}^3$ *satisfying* $\boldsymbol{F} = \mathsf{const}$ *and* (3.2) *with* $\rho = \langle x\rangle^m$, $\gamma = \langle x\rangle$, $m \in (-1, 0)$. *Then,*

(i) The asymptotics

$$\mathsf{N}_0^-(\eta) = \mathcal{N}^-(\eta) + O(\eta^{\frac{1}{m}-\delta}) \tag{6.3.6$_-$}$$

hold with

$$\mathcal{N}^-(\eta) = \frac{1}{2\pi^2}\int F(-V-\eta)_+^{\frac{1}{2}}\,dx \tag{3.8}$$

and arbitrarily small $\delta > 0$, *and furthermore,* $\mathcal{N}^-(\eta) = O(\eta^{\frac{3}{2m}+\frac{1}{2}})$. *Moreover,* $\mathcal{N}^-(\eta) \asymp \eta^{\frac{3}{2m}+\frac{1}{2}}$, *provided* $-V \geq \epsilon\rho^2$ *for* $x \in \Gamma$ *where* Γ *is a non-empty open cone in* $\mathbb{R}^3$.

(ii) Further, under the assumption

$$\sum_{|\alpha|\leq K} |\nabla^\alpha V|\cdot\gamma^{|\alpha|} \geq \epsilon\rho^2 \qquad \text{for } |x| \geq c, \tag{3.9}$$

the asymptotics (3.8) *hold with* $\delta = 0$.

Remark 3.4. (i) Similar results hold in the d-dimensional case when $(F_{jk}) = \mathsf{const}$ and $d > 2r = \mathsf{rank}(F_{jk})$: the remainder estimate is $O(\eta^{(d-2r-1)/2+(d-1)/2m-\delta})$ [42] and $\mathcal{N}^-(\eta) = O(\eta^{(d-2r)/2+d/2m})$.

(ii) Observe that for $m = -1$, both the principal part and the remainder estimate have magnitude η^{-r}.

(iii) One can also consider $\rho = \langle x\rangle^{-1}|\log\langle x\rangle|^{\alpha}$ with $\alpha > 0$.

For exact statements, details, proofs and generalizations, see Subsection 24.4.1 of [Ivr4].

Case $d > 2r$. II

We now discuss faster decaying potentials. Assume that $d = 2r+1$ (otherwise there will be no interesting results). Assume for simplicity that $g^{jk} = \delta_{jk}$ and $F_{dk} = 0$. Further, one can assume that $A_d(x) = 0$; otherwise one can achieve it by a gauge transformation. Then, $A_j = A_j(x')$ with $x' = (x_1, \dots, x_{2r})$ and the operator is of the form

$$D_d^2 + V(x) + H_0', \qquad \text{with} \quad H_0' := \sum_{1\le j\le d-1} (D_j - A_j(x'))^2. \tag{3.10}$$

For any fixed $x' : |x'| \ge c$, consider the one-dimensional operator

$$L := D_t^2 + V(x';t) \tag{3.11}$$

on $\mathbb{R} \ni t$. It turns out that under the assumption

$$|V(x';t)| \le \varepsilon t^{-2}, \tag{3.12}$$

with $\varepsilon \le (\frac{1}{4} - \epsilon)$, this operator has no more than one negative eigenvalue $\lambda(x')$; moreover, it has exactly one negative eigenvalue

$$\lambda(x') = -\frac{1}{4}W(x')^2 + O(\varepsilon^3), \tag{3.13}$$

provided

$$W(x') := \int_{\mathbb{R}} V(x';t) < 0 \qquad \text{and} \quad -W(x') \asymp \varepsilon. \tag{3.14}$$

[42] Where $\delta = 0$ if either $d \ge 2r+2$ or the assumption (3.9) is fulfilled.

Furthermore, in this case $\lambda(x')$ nicely depends on x'.

Let

$$|\nabla^\alpha V| \le c_\alpha \rho^2 \gamma_1^{-|\alpha'|}\gamma^{-\alpha_d}, \tag{3.15}$$

with $\rho = \langle x\rangle^l \langle x'\rangle^k$, $\gamma = \langle x\rangle$, $\gamma_1 = \langle x'\rangle$ and $l \le -2$, $m := 2l + 2k + 1 < 0$ and if

$$W(x') < 0, \qquad W(x') \asymp \rho', \qquad \rho' := \langle x'\rangle^m, \tag{3.16}$$

then we are essentially in the $(d-1)$-dimensional case of an operator $H' := H'_0 + \lambda(x')$, and for $\mathsf{N}^-(\eta)$, we have the corresponding asymptotics of Subsubsection 3.

For exact statements, details, proofs and generalizations, see Subsections 24.4.2 of [Ivr4]. For improvements for slower decaying potentials, see Subsections 24.4.3 of [Ivr4].

4 Applications to Multiparticle Quantum Theory

Problem Set-up

In this Chapter, we discuss an application to Thomas-Fermi Theory. Consider a large (heavy) atom or molecule; it is described by a *Multiparticle Quantum Hamiltonian*

$$\mathsf{H}_N = \sum_{1\le n\le N} H_V(x_n) + \sum_{1\le n<k\le N} \frac{1}{|x_n - x_k|} \tag{4.1}$$

where H is a *one-particle quantum Hamiltonian*, Planck constant $\hbar = 1$, electron mass $= \frac{1}{2}$, electron charge $= -1$. This operator acts on the space $\mathfrak{H} := \bigwedge_{1\le j\le N} \mathscr{L}^2(\mathbb{R}^3, \mathbb{C}^2)$ of totally antisymmetric functions $\Psi(x_1, \varsigma_1; \ldots; x_N, \varsigma_N)$ because the electrons are fermions, $x_n = (x_n^1, x_n^2, x_n^3)$ is a coordinate and $\varsigma_n \in \{-\frac{1}{2}, \frac{1}{2}\}$ is the *spin* of n-th particle. We identify the $\mathbb{C}^2$-valued function $\psi(x)$ on $\mathbb{R}^3$ with a scalar-valued function $\psi(x, \varsigma)$.

If the electrons did not interact between themselves, but the field potential was $-W(x)$, then they would occupy the lowest eigenvalues and the ground state wave functions would be the anti-symmetrized product

$\phi_1(x_1,\varsigma_1)\phi_2(x_2,\varsigma_2)\ldots\phi_N(x_N,\varsigma_N)$, where ϕ_n and λ_n are the eigenfunctions and eigenvalues of H_W respectively.

Then the local electron density would be $\rho_\Psi = \sum_{1\le n\le N}|\phi_n(x)|^2$ and according to the pointwise Weyl law (if there is no magnetic field)

$$\rho_\Psi(x) \approx \frac{1}{3\pi^2}(W+\nu)_+^{\frac{3}{2}}, \tag{4.2}$$

where $\nu = \lambda_N$. We first assume that there is no magnetic field and therefore, $H_V = -\Delta - V(x)$.

This density would generate the potential $-|x|^{-1}*\rho_\Psi$ and we would have $W \approx V - |x|^{-1}*\rho_\Psi$.

Replacing all approximate equalities by strict ones, we arrive to the *Thomas-Fermi equations*:

$$V - W^{\mathsf{TF}} = |x|^{-1}*\rho^{\mathsf{TF}}, \tag{4.3}$$

$$\rho^{\mathsf{TF}} = \frac{1}{3\pi^2}(W^{\mathsf{TF}}+\nu)_+^{\frac{3}{2}}, \tag{4.4}$$

$$\int \rho^{\mathsf{TF}}\,dx = N, \tag{4.5}$$

where $\nu \le 0$ is called the *chemical potential* and in fact approximates λ_N.

Considering atoms and molecules, we assume that

$$V(x) = \sum_{1\le m\le M}\frac{Z_m}{|x-\mathsf{y}_m|}, \tag{4.6}$$

where y_m is the *position* and Z_m is the *charge* of the m-th nuclei, M is fixed and $Z_1 \asymp Z_2 \asymp \ldots \asymp Z_M \asymp N \to \infty$.

Thomas-Fermi theory has been rigorously justified (with pretty good error estimates) and we want to explain how.

Reduction to One-Particle Problem

Estimate from below

We start from the estimate from below. The *ground state energy* $\mathsf{E}_N := \inf\langle \mathsf{H}_N\Psi,\Psi\rangle$, taken over all $\Psi\in\mathfrak{H}$ with $\|\Psi\| = 1$, where $\langle\cdot,\cdot\rangle$ denotes the inner product in $\mathfrak{H}$. Classical mathematical physics provides a wealth of results. One of them is the *electrostatic inequality* due to

E. H. Lieb [L]:

$$\sum_{1\le j<k\le N}\int |x_j-x_k|^{-1}|\Psi(x_1,\dots,x_N)|^2\,dx_1\cdots dx_N \ge \frac{1}{2}\mathsf{D}(\rho_\Psi,\rho_\Psi)-C\int\rho_\Psi^{\frac{4}{3}}(x)\,dx, \tag{4.7}$$

with ρ_Ψ defined by (4.2). This inequality holds for all (not necessarily antisymmetric) functions Ψ with $\|\Psi\|_{\mathscr{L}^2(\mathbb{R}^{3N})}=1$. Therefore,

$$\langle \mathsf{H}_N\Psi,\Psi\rangle \ge \sum_{1\le j\le N}\langle H_{V,x_j}\Psi,\Psi\rangle+\frac{1}{2}\mathsf{D}\big(\rho_\Psi,\rho_\Psi\big)-C\int\rho_\Psi^{\frac{4}{3}}(x)\,dx = \sum_{1\le j\le N}\langle H_{W,x_j}\Psi,\Psi\rangle+\frac{1}{2}\mathsf{D}\big(\rho_\Psi-\rho,\rho_\Psi-\rho\big)-\frac{1}{2}\mathsf{D}\big(\rho,\rho\big)-C\int\rho_\Psi^{\frac{4}{3}}(x)\,dx \tag{4.8}$$

and H_W is a one-particle Schrödinger operator with potential

$$W=V-|x|^{-1}*\rho, \tag{4.9}$$

where ρ is an arbitrarily chosen real-valued non-negative function and therefore,

$$(V-W,\rho_\Psi)=-\mathsf{D}(\rho,\rho_\Psi). \tag{4.10}$$

The physical sense of the second term in W is transparent: it is a potential created by the charge $-\rho$. Skipping the positive second term in the right-hand expression of (4.8) and believing that the last term is not very important for the ground state function Ψ [43)], we see that we need to estimate from below the first term. Since the first term is simply the sum of operators acting with respect to different variables, we can estimate it from below by

$$\langle (H_{W,x_j}-\nu)\Psi,\Psi\rangle+\lambda N \tag{4.11}$$

with arbitrary ν; therefore, it is bounded from below by $\mathsf{Tr}((H_W-\nu)_-)$, where $(H_W-\nu)_-$ denotes the negative part of the operator $(H_W-\nu)$, and hence its trace is the sum of the negative eigenvalues.

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43) When we derive the upper estimate for E, we will get an upper estimate for this term as a bonus.

Here, the assumption that Ψ is antisymmetric is crucial. Namely, for general (or symmetric–does not matter) Ψ, the best possible estimate is $\lambda_1 N$ where λ_1 is the lowest eigenvalue of H_W (we always assume that there are sufficiently many eigenvalues below the bottom of the essential spectrum of H_W) and we cannot apply semiclassical theory.

Thus we arrive to

$$\mathsf{E}_N \geq \operatorname{Tr}((H_W-\nu)_-) + \nu N - \frac{1}{2}\mathsf{D}\bigl(\rho,\rho\bigr) - CN^{\frac{5}{3}}, \tag{4.12}$$

where we used another result of E. H. Lieb [L]: $\int \rho_\Psi^{\frac{4}{3}}(x)\,dx \leq CN^{\frac{5}{3}}$ for the ground state Ψ.

Estimate from above

Here, we simply plug in a test function Ψ which is an (anti-symmetrized) product $\phi_1(x_1,\varsigma_1)\phi_2(x_2,\varsigma_2)\ldots\phi_N(x_N,\varsigma_N)$ where ϕ_n and λ_n are eigenfunctions and eigenvalues of H_W respectively, and we pick W later. It may happen, however, that H_W does not have N negative eigenvalues, then we can reduce N and use the inequality $\mathsf{E}_N \leq E_{N'}$ as $N' \leq N$.

Then, E_N is estimated from above by

$$\begin{aligned}\langle \mathsf{H}_N\Psi,\Psi\rangle = \\ \sum_n (H_{W,x_j}-\lambda)\Psi,\Psi\rangle + \lambda N - (V-W,\rho_\Psi) + \frac{1}{2}\mathsf{D}(\rho_\Psi,\rho_\Psi) \\ -\frac{1}{2}\sum_n \iint |x-y|^{-1}|\psi_n(x)|^2|\psi_n(y)|^2\,dxdy\end{aligned} \tag{4.13}$$

and therefore recalling (4.10), we obtain

$$\mathsf{E}_N \leq \operatorname{Tr}((H_W-\lambda)_-) + \lambda N + \frac{1}{2}\mathsf{D}(\rho_\Psi-\rho,\rho_\Psi-\rho) - \frac{1}{2}\mathsf{D}(\rho,\rho) \tag{4.14}$$

and $\rho_\Psi = \operatorname{tr} e_N(x,x)$ where $e_N(x,y)$ and $e(x,y,\lambda)$ are the Schwartz kernels of the projector to the N lowest eigenvalues of H_W and of the operator $\theta(\lambda - H_W)$ respectively; here tr denotes the matrix trace, and $\lambda=\lambda_N$ if $\lambda_N<0$ and $\lambda=0$ otherwise. Finally, we conclude that

$$\begin{aligned}\mathsf{E}_N \leq \operatorname{Tr}((H_W-\nu)_-) + \nu N + |\lambda-\nu|\cdot|\mathsf{N}^-(H_W-\nu)-N| \\ + \frac{1}{2}\mathsf{D}(\operatorname{tr} e_N(x,x)-\rho,\operatorname{tr} e_N(x,x)-\rho) - \frac{1}{2}\mathsf{D}(\rho,\rho)\end{aligned} \tag{4.15}$$

with arbitrary $\nu \leq 0$.

Semiclassical Approximation

Estimate from below

In the estimate from below (4.12), we replace $\mathsf{Tr}((H_W-\nu)_-)$ by its semiclassical approximation

$$\mathsf{Tr}((H_W-\nu)_-)\approx -\int P(W+\nu)\,dx \tag{4.16}$$

with

$$P(W+\nu):=\frac{2}{5\pi^2}(W+\nu)_+^{\frac{5}{2}}, \tag{4.17}$$

and also plug in $\rho=\frac{1}{4\pi}\Delta(W-V)$; then we obtain the functional

$$\Phi_*(W,\nu)=-\int P(W+\nu)\,dx-\frac{1}{8\pi}\|\nabla(W-V)\|^2+\nu N; \tag{4.18}$$

maximizing it, we arrive to the Thomas-Fermi equations and its maximal value is $\mathcal{E}_N^{\mathsf{TF}}$, delivered by Thomas-Fermi theory. Then, we need to understand the semiclassical error. To do this, we use the properties of the Thomas-Fermi potential and rescale $x\mapsto xN^{\frac{1}{3}}$ and $\tau\mapsto N^{-\frac{4}{3}}\tau$ (so, $\nu\mapsto N^{-\frac{4}{3}}\nu$) with

$$H_W=-h^2\nabla^2-W, \tag{4.19}$$

where near y_m, the rescaled potential is Coulomb-like: $W\sim z_m|x-y|^{-1}$ with $z_m=Z_mN^{-1}$.

Then, we can apply results Subsection 3 (see (3.53)): for the operator (4.19),

$$\mathsf{Tr}((H_W-\nu)_-)=-h^{-3}\int P(W+\nu)\,dx+\kappa h^{-2}+O(h^{-1}), \tag{4.20}$$

where in this case, the numerical value of $\kappa=2\sum_m z_m^2$ is well-known. Scaling back, we obtain $\mathcal{E}_N^{\mathsf{TF}}+\mathsf{Scott}+O(N^{\frac{5}{3}})$ where the leading term is of magnitude $N^{\frac{7}{3}}$ and the Scott correction term $\mathsf{Scott}=2\sum_m Z_m^2$. Here, we need to assume that $|\mathsf{y}_m-\mathsf{y}_{m'}|\gtrsim 1$ after rescaling (and $|\mathsf{y}_m-\mathsf{y}_{m'}|\gtrsim N^{-\frac{1}{3}}$ before it).

Indeed, after rescaling, we get an operator which is uniformly in the framework of Subsection 3 due to the following properties of the Thomas-Fermi potential:

(4.21) Before rescaling, $W^{\mathsf{TF}} = Z_m|x-\mathsf{y}_m|^{-1} + O(N)$ for $|x-\mathsf{y}_m| \lesssim N^{-\frac{1}{3}}$ and $W^{\mathsf{TF}} \asymp \sum_m \bigl(|x-\mathsf{y}_m|^{-4} + (Z-N)_+|x-\mathsf{y}_m|^{-1}\bigr)$ for $|x-\mathsf{y}_m| \gtrsim 1$ for all $m=1,\dots,M$.

In fact, the analysis of Subsection 3 was mainly motivated by this problem.

Estimate from above

Again, using the semiclassical approximation (4.16) for $\operatorname{Tr}((H_W-\nu)^-)$ and also $e_N(x,x) \approx P'(W+\nu)$ with $P' = \frac{1}{3\pi^2}(W+\nu)^{\frac{3}{2}}$ the derivative of $P(W+\nu)$, we arrive to the functional

$$\begin{aligned}\Phi^*(W,\nu) = -\int P(W+\nu)\,dx - \frac{1}{8\pi}\|\nabla(W-V)\|^2 + \nu N \\ + \mathsf{D}\Bigl(P'(W+\nu) - \frac{1}{4\pi}\Delta(W-V),\ P'(W+\nu) - \frac{1}{4\pi}\Delta(W-V)\Bigr);\end{aligned} \tag{4.22}$$

minimizing it, we again arrive to the Thomas-Fermi equations and the minimal value is $\mathcal{E}_N^{\mathsf{TF}}$, again delivered by Thomas-Fermi theory.

However, in addition to the semiclassical error for the trace, we have other errors from (4.15):

$$|\lambda-\nu|\cdot|\mathsf{N}^-(H_W-\nu)-N|, \tag{4.23}$$

$$\mathsf{D}\bigl(\operatorname{tr} e(x,x,\nu) - P'(W+\nu),\ \operatorname{tr} e(x,x,\nu) - P'(W+\nu)\bigr) \tag{4.24}$$

and

$$\mathsf{D}\bigl(\operatorname{tr} e_N(x,x) - \operatorname{tr} e(x,x,\nu),\ \operatorname{tr} e_N(x,x) - \operatorname{tr} e(x,x,\nu)\bigr). \tag{4.25}$$

The expression (4.24) is the semiclassical error and after rescaling it, we can estimate it by $O(h^{-4})$ (due to the pointwise spectral asymptotics). When scaling back, we gain the factor $N^{\frac{1}{3}}$, resulting in $O(N^{\frac{5}{3}})$.

Expressions (4.23) and (4.25) can be also estimated by $O(N^{\frac{5}{3}})$ based on another semiclassical error

$$\mathsf{N}^-(H_W-\sigma) - \int P'(W+\sigma)\,dx = O(h^{-2}), \tag{4.26}$$

(for $\sigma \le 0$) after rescaling and thus, $O(N^{\frac{2}{3}})$ in the original scale, due to the definitions of λ and ν. One needs to consider four cases depending on whether $\lambda<0$ (i.e. $N^-(H_W) \ge N$) or $\lambda=0$ (i.e. $N^-(H_W) < N$) and whether $\nu<0$ (i.e. $N<Z$) or $\nu=0$ (i.e. $N \ge Z$), where $Z = Z_1+\dots+Z_M$ is the total charge of the nuclei.

More Precise Estimates

If we want to improve the remainder estimate $O(N^{\frac{5}{3}})$, then we need to improve the semiclassical remainder estimates and also deal with $O(N^{\frac{5}{3}})$ in Lieb's electrostatic inequality (4.7).

The first task could be done under the assumption

$$a := \min_{m\neq m'} |\mathsf{y}_m - \mathsf{y}_{m'}| \gg \bar{a} := N^{-\frac{1}{3}}, \tag{4.27}$$

which is completely reasonable (see Section 4). In this case, in each zone $\mathcal{Y}_m := \{x:\ |x-\mathsf{y}_m| \le a^{1-\eta}\bar{a}^{\eta}\}$, with $\eta > 0$, both ρ^{TF} and W^{TF} are close to those of a single atom which are spherically symmetric. Then one can prove easily that the standard conditions to the trajectories are fulfilled and we may use the improved remainder estimates. On the other hand, contributions of the "outer" zone $\mathcal{Y}_0 := \{x:\ |x-\mathsf{y}_m| \ge a^{1-\eta}\bar{a}^{\eta}\ \forall m = 1,\dots,M\}$ to these remainders is smaller.

Therefore all remainder estimates acquire the factor $(h^{\delta} + b^{-\delta})$ with $b = a\bar{a}^{-1}$ before scaling back, i.e. $(N^{\frac{1}{3}\delta} + (aN^{\frac{1}{3}})^{-\delta})$ after it. However, the trace asymptotics should also include the term $-\kappa_1 h^{-1}$ before scaling back or $-\kappa_1 N^{\frac{5}{3}}$ after it; for the potential W^{TF}, it is numerically equal to $\mathsf{Schwinger} = -c_1\int \rho^{\mathsf{TF}\,\frac{4}{3}}\,dx$ which is called the *Schwinger correction term.*

The second task requires an improvement in Lieb's electrostatic inequality due to [GS] and [Ba]: one can replace the last term in (4.8) for the ground state energy Ψ by

$$-\frac{1}{2}\iint |x-y|^{-1}\operatorname{tr}\bigl(e_N^{\dagger}(x,y)e_N(x,y)\bigr)\,dxdy - O(N^{\frac{5}{3}-\delta}), \tag{4.28}$$

where the first term coincides with the last term in (4.13) (the estimates from above) and again modulo $O(N^{\frac{5}{3}-\delta})$ can be rewritten as

$$-\frac{1}{2}\iint |x-y|^{-1}\operatorname{tr}\bigl(e^{\dagger}(x,y,\nu)e(x,y,\nu)\bigr)\,dxdy. \tag{4.29}$$

So far, we have not explored such expressions but we can handle them.

For this expression, after rescaling, we can derive the asymptotics with principal term $-\kappa_2 h^{-4}$ and with remainder estimate as good as $O(h^{-3})$, which after scaling back becomes $O(N^{\frac{4}{3}})$ (which is an overkill). Here, we use the representation of $e(x,y,\nu)$ by an oscillatory integral modulo a term whose $\mathscr{L}^2(\mathbb{R}^6)$ norm does not exceed Ch^{-2}.

To calculate κ_2, we can consider the operator with constant potential W, and for this operator, we calculate $-\frac{1}{2}\int |x-y|^{-1}\operatorname{tr}\bigl(e^\dagger(x,y,\nu)e(x,y,\nu)\bigr)\,dy$ obtaining $-\mathsf{const}(W+\nu)^2h^{-4}$, then plug in $W=W(x)$ and integrate over x. For $W=W^{\mathsf{TF}}$, after scaling back, we arrive to $\mathsf{Dirac}=-c_2\int \rho^{\mathsf{TF}\,\frac{4}{3}}\,dx$ which is called the *Dirac correction term.*

Despite having completely different origins, these correction terms differ only by numerical constants.

We arrive to the theorem:

Theorem 4.1. *As* $Z=Z_1+\ldots+Z_M\asymp N\to\infty$, M *remains bounded,* $a=\min_{m\neq m'}|\mathsf{y}_m-\mathsf{y}_{m'}|\gtrsim N^{-\frac{1}{3}}$ *and*

$$\mathsf{E}_N=\mathcal{E}_N^{\mathsf{TF}}+\mathsf{Scott}+\mathsf{Schwinger}+\mathsf{Dirac}+O(R) \qquad \text{with}\quad R=N^{\frac{5}{3}}\bigl(N^{-\delta}+(aN^{\frac{1}{3}})^{-\delta}\bigr) \tag{4.30}$$

where $\delta>0$ *is unspecified.*

As a byproduct of the proof, we obtain

$$\mathsf{D}(\rho_\Psi-\rho^{\mathsf{TF}},\,\rho_\Psi-\rho^{\mathsf{TF}})=O(R). \tag{4.31}$$

For details and proofs, see Sections 25.1–25.4 of [Ivr4].

Ramifications

First, instead of the *fixed nuclei model*, we can consider the *free nuclei model* where we add to both E_N and $\mathcal{E}_N^{\mathsf{TF}}$ the energy of nuclei-to-nuclei interaction

$$\sum_{m<m'} Z_mZ_{m'}|\mathsf{y}_m-\mathsf{y}_{m'}|^{-1} \tag{4.32}$$

and minimize the results by the position of nuclei $(\mathsf{y}_1,\ldots,\mathsf{y}_m)$; denote the results by $\widehat{\mathsf{E}}_N$ and $\widehat{\mathcal{E}}_N^{\mathsf{TF}}$ respectively.

Combining (4.30) with the non-binding theorem in Thomas-Fermi theory[44], we obtain that in the free nuclei model (with $Z_1\asymp\ldots\asymp Z_M\asymp Z\asymp N$),

$$a=\min_{m\neq m'}|\mathsf{y}_m-\mathsf{y}_{m'}|\gtrsim N^{-\frac{5}{3}+\delta} \tag{4.33}$$

and then (4.30) and (4.31) hold with $R=N^{\frac{5}{3}-\delta}$.

[44] In the Thomas-Fermi theory, molecules do not exist.

Next, using methods already developed by mathematical physicists before asymptotics (4.30) and (4.31) were derived, we can answer several questions with far better precision than before; for simplicity, we assume that $a \geq N^{-\frac{1}{3}+\delta}$.

(i) How many extra electrons can the system bind? In other words, if $\mathsf{E}_N < \mathsf{E}_{N-1}$, what we can say about $N-Z$? According to a classical theorem due to G. Zhislin, the system can bind at least Z electrons. Our answer: $(N-Z)_+ = O(N^{\frac{5}{7}-\delta})$, based on the fact that in the Thomas-Fermi theory, negative ions do not exist.

(ii) What we can say about the *ionization energy* $\mathsf{I}_N = \mathsf{E}_{N-1} - \mathsf{E}_N$? Our answer: $\mathsf{I}_N = O(N^{\frac{20}{21}-\delta})$ if $N-Z \geq -CN^{\frac{5}{7}-\delta}$ and $\mathsf{I}_N = -\nu + O((Z-N)^{\frac{17}{18}} Z^{\frac{5}{18}-\delta}$ if $N-Z \leq -CN^{\frac{5}{7}-\delta}$; if $N \leq Z$ $\nu \asymp (Z-N)^{\frac{4}{3}}$.

(iii) In the free nuclei model (with $M \geq 2$), what can we say about $N-Z > 0$ if a stable configuration exists? Our answer: $Z - N \leq CN^{\frac{5}{7}-\delta}$ (again based on the non-binding theorem).

For details and proofs, see Sections 25.5 and 25.6 of [Ivr4].

Adding Magnetic Field

Adding External Magnetic Field

Consider the Schrödinger-Pauli operator with magnetic field

$$H_{A,V} = ((-ih\nabla - \mu A(x)) \cdot \boldsymbol{\sigma})^2 - V(x). \tag{4.34}$$

Then instead of $P(w)$ defined by (4.17), we need to define it according to (2.5) by

$$P(w) = \frac{2}{\pi^2}\Bigl(\frac{1}{2} w_+^{\frac{3}{2}} B + \sum_{j=1}^{\infty} (w - 2jB)_+^{\frac{3}{2}} B\Bigr), \tag{4.35}$$

where B is the scalar intensity of the magnetic field. This changes both the Thomas-Fermi theory and properties of the Thomas-Fermi potential W^{TF} and Thomas-Fermi density ρ^{TF}.

Case $B \lesssim Z^{4/3}$ For $B \lesssim Z^{4/3}$, the main contributions to the (approximate) electronic charge $\int \rho^{\mathsf{TF}}\,dx$ and the energy $\mathcal{E}^{\mathsf{TF}}$ come from the zone $\{x : d(x) \asymp Z^{-1/3}\}$ ($d(x) = \min_m |x - \mathsf{y}_m|$), exactly as for $B = 0$.

Furthermore, $W^{\mathsf{TF}} \asymp Z_m d(x)^{-1}$ if $d(x) \lesssim Z^{-1/3}$ and (for $Z = N$) $W^{\mathsf{TF}} \asymp d(x)^{-4}$ if $Z^{-1/3} \le d(x) \lesssim B^{-1/4}$ but $\rho^{\mathsf{TF}} = 0$ if $d(x) \ge C_0 B^{-1/4}$ [45].

Finally, as we using scaling to bring our problem to the standard one, we get that in the zone $\{x : d(x) \asymp Z^{-1/3}\}$, the effective semiclassical parameter is $h_{\mathsf{eff}} = Z^{-1/3}$ which leads to $\mathcal{E}^{\mathsf{TF}} \asymp Z^{7/3}$ again exactly as for $B = 0$.

As a result, assuming that $M = 1$, we can recover asymptotics for the ground state energy E with the Scott correction term but with the remainder estimate $O(Z^{5/3} + Z^{4/3}B^{1/3})$. For $M \ge 2$ and $N \ge Z$, our estimates are almost as good (provided $a = \min_{m \ne m'} |\mathsf{y}_m - \mathsf{y}_{m'}| \ge Z^{-1/3}$), but deteriorate when both $(Z - N)_+$ and B are large.

Moreover, for $B \ll Z$ assuming (4.27), we can marginally improve these results and include the Schwinger and Dirac correction terms.

The main obstacles we need to overcome are that now W^{TF} is not infinitely smooth but only belongs to the class $\mathscr{C}^{5/2}$ and that for $M \ge 2$, the nondegeneracy assumption ($|\nabla W| \asymp 1$ after rescaling) fails.

Case $B \gtrsim Z^{4/3}$ On the other hand, for $B \gtrsim Z^{4/3}$, the the main contributions to the (approximate) electronic charge and the energy $\mathcal{E}^{\mathsf{TF}}$ come from the zone $\{x : d(x) \asymp B^{-1/4}\}$ and (for $Z = N$) $W^{\mathsf{TF}} \asymp Zd(x)^{-1}$ if $d(x) \lesssim B^{-1/4}$ but $W^{\mathsf{TF}} = 0$ if $d(x) \ge C_0 B^{-1/4}$. In this case, $\mathsf{E}^{\mathsf{TF}} \asymp B^{2/5} Z^{9/5}$.

Further, as we using scaling to bring our problem to the standard one, we see that in the zone $\{x : d(x) \asymp B^{-1/4}\}$, the effective semiclassical parameter is $h_{\mathsf{eff}} = B^{1/5} Z^{-3/5}$ and therefore unless $B \ll Z^3$, the semiclassical approximation fails and the correct answer should be expressed in completely different terms [LSY1].

As a result, assuming that $M = 1$ if $Z^{4/3} \le B \le Z^3$, we can recover the asymptotics for E with the Scott correction term but with the remainder estimate $O(B^{4/5} Z^{3/5} + Z^{4/3} B^{1/3})$.

For $M \ge 2$ and $N \ge Z$, our estimates are almost as good (provided $a = \min_{m \ne m'} |\mathsf{y}_m - \mathsf{y}_{m'}| \ge B^{-1/4}$), but deteriorate when $(Z - N)_+$ is large.

Again the main obstacles we need to overcome are that now W^{TF} is not infinitely smooth but only belongs to $\mathscr{C}^{5/2}$ and that for $M \ge 2$, the nondegeneracy assumption ($|\nabla W| \asymp 1$ after rescaling) fails.

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[45] So, the radii of atoms in Thomas-Fermi theory are $\asymp \min(B^{-1/4}, (Z - N)_+^{-1/3})$.

For details, exact statement and proofs, see Sections 26.1 and 26.6 of [Ivr4]. We also estimate the left-hand expression of (4.20) and are able to obtain results similar to those mentioned in Section 4. For details and proofs, see Sections 26.7–26.8 of [Ivr4].

Adding Self-Generated Magnetic Field

Let

$$\mathsf{E}(A) = \inf \operatorname{Spec}(\mathsf{H}_{A,V}) + \underline{\alpha^{-1} \int |\nabla \times A|^2\, dx} \tag{4.36}$$

and

$$\mathsf{E}^* = \inf_{A\in\mathscr{H}^1_0} \mathsf{E}(A), \tag{4.37}$$

where A is an unknown magnetic field and the underlined term is its energy. One can prove that an "optimal" magnetic field exists (for given parameters $Z_1, \dots, Z_M, \mathsf{y}_1, \dots, \mathsf{y}_M, N$) but we do not know if it is unique[46].

Using the same arguments as before, we can reduce this problem to the one-particle problem with $\inf \operatorname{Spec}(\mathsf{H}_{A,V})$ replaced by $\operatorname{Tr}((H_{A,W}+\nu)_-)$ plus some other terms. However, in the estimate from below, most of the terms do not depend on A and in the estimate from above, we pick up A.

Then after the usual rescalings, the problem is reduced to the problem of minimizing

$$\operatorname{Tr}((H_{A,W}+\nu)_-) + \underline{\frac{1}{\kappa h^2} \int |\nabla \times A|^2\, dx} \tag{4.38}$$

and then the optimal magnetic potential A must satisfy

$$\begin{aligned} \frac{2}{\kappa h^2}\Delta A_j(x) = \Phi_j :=& \\ -\operatorname{Re}\operatorname{tr}\Bigl(\sigma_j\Bigl((hD-A)_x\cdot \boldsymbol{\sigma} e(x,y,\tau) &+ e(x,y,\tau)\,{}^t(hD-A)_y\cdot\boldsymbol{\sigma}\Bigr)\Bigr|_{y=x}\Bigr), \end{aligned} \tag{4.39}$$

where $e(x,y,\tau)$ is the Schwartz kernel of the spectral projector $\theta(-H)$ of $H=H_{A,W}$ and tr is the matrix trace. As usual, we are mainly interested in $h=Z^{-1/3}$ (and then $\kappa=\alpha Z$).

[46] If it was unique, then for $M=1$, the spherical symmetry would imply that $A=0$.

First, (4.39) allows us to claim a certain smoothness of A. Second, the right-hand expression is something we studied in pointwise spectral asymptotics, and the Weyl expression here is 0, so the right-hand expression of (4.39) is something that we could estimate. Surely, it is not that simple but improving our methods in the case of smooth W, we are able to prove that A is so small that the ordinary asymptotics with remainder estimates $O(h^{-2})$ and $O(h^{-1})$ would hold in both the pointwise asymptotics and the trace asymptotics. Moreover, under standard conditions, we would be able to get the remainder estimates $o(h^{-2})$ and $o(h^{-1})$ in the eigenvalue counting and the trace asymptotics respectively.

However, in reality, the above is not exactly true since W has Coulomb-like singularities $W \sim z_m|x - y_m|^{-1}$ with $z_m \asymp 1$. If $M = 1$, $z_m = 1$, a singularity leads us to the Scott correction term $S(\kappa)h^{-2}$ derived in the same way as without a self-generated magnetic field. However, we do not have an explicit formula for $S(\kappa)$; we even do not know its properties except that it is non-increasing function of $\kappa \in [0, \kappa^*)$; we even do not know if we can take $\kappa^* = \infty$. If the optimal magnetic potential A was unique, then $A = 0$ and $S(\kappa) = S(0)$, which corresponds to this term without a magnetic field.

Then as $M \geq 2$, the Scott correction term is $\sum_{1\leq m\leq M} S(\kappa z_m)z_m^2 h^{-2}$ in the general case. However, as $M \geq 2$ we need to decouple singularities as all of them are served by the same A and it leads to decoupling errors depending on the internuclei distance.

For details, exact statements and proofs, see Sections 27.2–27.3 of [Ivr4].

As a result, we derive the ground state asymptotics with the Scott correction term $\sum_{1\leq m\leq M} S(\alpha Z_m)Z_m^2$. We also estimate the left-hand expression of (4.20) and are able to obtain results similar to those mentioned in Section 4. For details, exact statements and proofs, see Sections 27.3–27.4 of [Ivr4].

Combining External and Self-Generated Magnetic Fields

We can also combine a constant strong external magnetic field and a self-generated magnetic field. Results are very similar to those of Subsection 4, but this time, the Scott correction term and the decoupling errors are like in Subsection 4. For details, exact statements and proofs, see Chapter 28 of [Ivr4].

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Presentations

[1] *Sharp spectral asymptotics for irregular operators*

[2] *Sharp spectral asymptotics for magnetic Schrödinger operator*

[3] *25 years after*

[4] *Spectral asymptotics for 2-dimensional Schrödinger operator with strong degenerating magnetic field*

[5] *Magnetic Schrödinger operator: geometry, classical and quantum dynamics and spectral asymptotics*

[6] *Spectral asymptotics and dynamics*

[7] *Magnetic Schrödinger operator near boundary*

[8] *2D- and 3D-magnetic Schrödinger operator: short loops and pointwise spectral asymptotics*

[9] *100 years of Weyl's law*

[10] *Some open problems, related to spectral theory of PDOs*

[11] *Large atoms and molecules with magnetic field, including self-generated magnetic field (results: old, new, in progress and in perspective)*

[12] *Semiclassical theory with self-generated magnetic field*

[13] *Eigenvalue asymptotics for Dirichlet-to-Neumann operator*

[14] *Eigenvalue asymptotics for Fractional Laplacians*

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[18] *Complete semiclassical spectral asymptotics for periodic and almost periodic perturbations of constant operators*

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