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Essays in Honor o

Lennart Carleson's

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Perspectives in Analysis

Essays in Honor of Lennart Carleson's 75th Birthday

Edited by

Michael Benedicks
Peter W. Jones
Stanislav Smirnov

Springer

Editors

Michael Benedicks

Royal Institute of Technology
Department of Mathematics
S-100 44 Stockholm, Sweden
e-mail: michaelb@kth.se

Peter W. Jones

Yale University
Department of Mathematics
10 Hillhouse Ave
P.O. Box 208283
New Haven, CT 06520-8283, U.S.A.
e-mail: jones-peter@yale.edu

Stanislav Smirnov

Royal Insitute of Technology
Department of Mathematics
S-100 44 Stockholm, Sweden

and

Université de Genève
Section de Mathématiques
2-4, rue du Lièvre
1211 Genève 4, Switzerland
e-mail: stas@kth.se

Technical Editor

Björn Winckler

University of Groningen
Department of Mathematics
P.O. Box 800
9700 AV Groningen, The Netherlands
e-mail: winckler@kth.se

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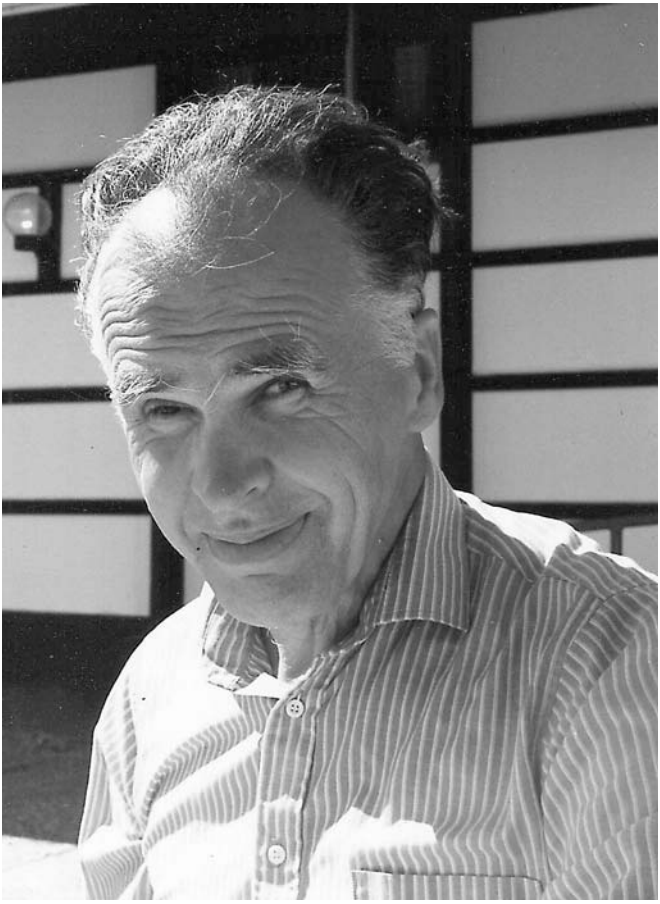

This book is dedicated to Lennart Carleson
on the occasion of his 75th birthday

Preface

The Conference “Perspectives in Analysis” was held during May 26–28, 2003 at the Royal Institute of Technology in Stockholm, Sweden. The purpose of the conference was to consider the future of analysis along with its relations to other areas of mathematics and physics, and to celebrate the seventy-fifth birthday of Lennart Carleson. The scientific theme was one with which the name of Lennart Carleson has been associated for over fifty years. His modus operandi has long been to carry out a twofold approach to the selection of research problems. First one should look for promising new areas of analysis, especially those having close contact with physically oriented problems of geometric character. The second step is to select a core set of problems that require new techniques for their resolutions. After making a central contribution, Lennart would usually move on to a new area, though he might return to the topic of his previous work if new techniques were developed that could break old mathematical log jams. Lennart’s operating approach is based on fundamental realities of modern mathematics as well as his own inner convictions. Here we first refer to an empirical fact of mathematical research: All topics have a finite half-life, with fifteen years being an upper bound for most areas. After that time it is usually a good idea to move on to something new. Secondly, the divorce between mathematics and physics, though never complete, was a disaster for analysis in the middle of the twentieth century. Physics and physical intuition have always led to many of the deepest advances in analysis. The past two and a half decades have seen analysis become increasingly dominated by this philosophy once again, with areas such as Stochastic Loewner Evolutions and critical lattice models, both of which have deep ties to conformal field theory, being in the vanguard over the past five years. Lennart has been a forceful advocate of both these newer areas as well as a recurrent theme of his own research: Find and explain the fundamental mechanisms underlying the behavior exhibited in key physical features of a problem. This, however, was only the first step for his work in an area. The other crucial aspect of his lifework has been to discover young talents and nurture the brightest of these. This step could not be taken without developing an international group of experts covering many aspects of analysis. There were then conferences and programs to be arranged, and Lennart has also spent enormous time on this aspect of mathematics.

After completing high school in 1945, Lennart started his college studies in Uppsala, where he continued with his graduate studies. With the mercurial genius Arne Beurling as his thesis advisor, Lennart rapidly struck out on his own. His 1950 thesis on Sets of Uniqueness led to important results published in Acta Mathematica. Continuing his research in complex analysis, in the late 1950's he classified the interpolating sequences for bounded analytic functions on the disk. Here the key idea was the introduction of what is now a cornerstone of modern analysis, namely Carleson Measures. (Lennart's name for these was much more prosaic.) This led a few years later to his solution of the Corona Problem for the disk. It is interesting to note that after this solution of a famous, long-standing conjecture, Lennart turned his attention to other areas, basically leaving corona problems until the early 1980's, when new methods led him to return and prove an extension of the Corona theorem for the case of uniformly thick Denjoy domains. Instead Lennart turned his attention to the Lusin conjecture on almost everywhere convergence of Fourier series for L^2 functions. His celebrated solution, published in Acta Mathematica in 1966, is regarded as one of the greatest accomplishments in analysis during the twentieth century. The technical difficulty of this result is hard to overstate and it is only within the past few years that almost everywhere convergence has been more fully integrated with the rest of the machinery of harmonic analysis. In the 1970's one of Lennart's fundamental contribution was to prove the Lifting Theorem for quasiconformal mappings in the case of $\mathbb{R}^3$ to $\mathbb{R}^4$. Lifting from $\mathbb{R}$ to $\mathbb{R}^2$ had been proven by Ahlfors and Beurling, and Ahlfors had later handled the case for $\mathbb{R}^2$ to $\mathbb{R}^3$. The key idea in Carleson's theorem was to replace the complex analytic methods of Ahlfors (using quasiconformal factorization) and find an extension by applying the philosophy of Beurling–Ahlfors plus a complicated geometric innovation. (This led several years later to a full solution of the Lifting Problem by Tukia and Väisälä.) In the 1980's there was a reblossoming of interest in dynamical systems and Lennart turned his attention there. (Few remember that in the 1960's Lennart had been the advisor for H. Brolin's thesis, which introduced the Brolin potential for polynomial Julia sets.) In a paper with M. Benedicks, he gave a new proof of Jacobson's theorem on chaotic behavior of $x^2 + a$, for positive measure of parameters $a \in (-2, -2 + \varepsilon)$. The new feature here was a powerful combinatorial argument on forward images of intervals and how these images behaved when they came near the origin. In a later paper Carleson and Benedicks found a far-reaching extension that allowed them to prove the existence of a Cantor set of positive measure (in parameter space) where the associated Hénon map has a strange attractor. It seems that Lennart's focus is always on the newest problem or area of research, and what comes next from him we cannot guess.

Lennart's devotion to mathematics is not limited to his mathematical output and influence. He has worked tirelessly for the promotion of international cooperation in mathematics. In the late 1960's he restarted the Institut Mittag-Leffler, which had been more or less moribund since the death of Mittag-Leffler in the 1920's. He served as its director until the 1984, leaving it in its present status as a jewel of Swedish mathematics and a world center of research. In the early 1980's, at a time of great international tensions, Lennart served as president of the International Mathematical Union. In its most difficult hour, when the political circumstances of 1982 led to postponement of the (quadrennial) International Congress, Lennart provided the leadership to bring off a successful Congress one year later. These two accomplishments give only a hint of Lennart's work; he was one of the past century's most influential leaders in the cause of furthering international cooperation in mathematics.

With this background in mind, the 2003 conference on Perspectives in Mathematics was planned with the theme of new and developing directions in analysis. Experts from a wide spectrum of the analysis world presented their visions or prognostications for the future. Our hope is that these proceedings will provide a source of inspiration for the new generation of analysts, and that Lennart will accept this volume as a small token of affection from his many devoted friends all over the world of mathematics.

The conference was made possible due to the generosity of the Swedish Foundation for International Cooperation in Research and Higher Education (STINT), the Swedish Research Council (Vetenskapsrådet), and the Göran Gustafssons Foundation. We thank them very much for their support. We also thank Björn Winckler for his excellent work as technical editor of this volume and the accompanying DVD.

Stockholm, Sweden,
February 2005

Michael Benedicks
Peter W. Jones
Stanislav Smirnov

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List of Contributors

Enrico Bombieri
Institute for Advanced Study
School of Mathematics
Princeton, NJ 08540, USA
eb@math.ias.edu

J. Bourgain
Institute for Advanced Study
School of Mathematics
Princeton, NJ 08540, USA
bourgain@math.ias.edu

R.R. Coifman
Department of Mathematics
Yale University
New Haven, CT 06520, USA
coifman@math.yale.edu

Guy David
Équipe d'Analyse Harmonique (CNRS)
Université de Paris XI (Paris-Sud)
91405 Orsay, France
guy.david@math.u-psud.fr

Björn Engquist
KTH, Nada
SE-100 44 Stockholm, Sweden
engquist@nada.kth.se
and Department of Mathematics
University of Texas at Austin
Austin, TX 78712-1082, USA
engquist@ices.utexas.edu

L. D. Faddeev
St. Petersburg Department of
Steklov Mathematical Institute
St. Petersburg, Russia
faddeev@pdmi.ras.ru

Lars Gårding
University of Lund, Sweden
Lars.Garding@math.lu.se

Peter W. Jones
Department of Mathematics
Yale University
New Haven, CT 06520, USA
jones-peter@yale.edu

Jean-Pierre Kahane
Département de mathématiques
Université Paris-Sud
Orsay Bât. 425
F-91405 Orsay Cedex, France
jean-pierre.kahane@math.u-psud.fr

Elliott H. Lieb
Departments of Mathematics and Physics
Princeton University
Jadwin Hall P.O. Box 708
Princeton, NJ 08544, USA
lieb@math.princeton.edu

N. Makarov
California Institute of Technology
Department of Mathematics
Pasadena, CA 91125, USA
makarov@its.caltech.edu

Paul Malliavin
10 rue Saint Louis en l'Isle
75004 Paris, France
sli@ccr.jussieu.fr

A. Poltoratski
Texas A&M University
Department of Mathematics
College Station, TX 77843, USA
alexeip@math.tamu.edu

Robert Seiringer
Department of Physics
Princeton University
Jadwin Hall, P.O. Box 708
Princeton, NJ 08544, USA
rseiring@math.princeton.edu

Ya. G. Sinai
Mathematics Department
Princeton University USA
and Landau Institute of Theoretical Physics
Russian Academy of Sciences
sinai@math.princeton.edu

Jan Philip Solovej
Institute for Advanced Study
School of Mathematics
Princeton, NJ 08540, USA
On leave from Dept. of Math.
University of Copenhagen
Universitetsparken 5
DK-2100 Copenhagen, Denmark
solovej@math.ku.dk

Nicholas Th. Varopoulos
Université Pierre & Marie Curie – Paris VI
and Institut Universitaire de France
Département de Mathématiques
75252 Paris Cedex 05, France
vnth2003@yahoo.ca

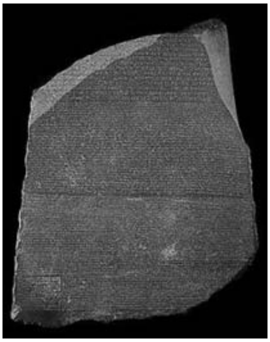
Jakob Yngvason
Institut für Theoretische Physik
Universität Wien
Boltzmanngasse 5
A-1090 Vienna, Austria
yngvason@thor.thp.univie.ac.at

The Rosetta Stone of L-functions

Enrico Bombieri

Institute for Advanced Study, School of Mathematics, Princeton, NJ 08540, USA
eb@math.ias.edu

THE ROSETTA STONE



The Rosetta stone (1808)
British Museum

The Rosetta Stone carries an identical text with parallel inscriptions in hieroglyphs, demotic and Greek. It is associated with the famous egyptologist Champollion (1790–1832), who used it, after he had deciphered demotic, as the starting point for reading hieroglyphs. He recognized on the Rosetta stone the name Ptolmys in Greek and demotic, and from there he identified the same name in hieroglyphs, written in a cartouche. Three years later, in 1821, while studying corresponding hieroglyphic and Greek texts on an obelisk transported to England by Giovanni Belzoni (1778–1823), he recognized the name Kliopadra, thus getting the values of twelve hieroglyphs. From there, he was able to complete the monumental task he had started in 1808 at the age of eighteen.

ZETA AND L-FUNCTIONS [13]

Number fields. The Dedekind zeta function of a number field K is defined by

$$\zeta_K(s) = \sum_{\mathfrak{a}} \frac{1}{N(\mathfrak{a})^s} = \prod_{\mathfrak{p}} \Big(1 - \frac{1}{N(\mathfrak{p})^s}\Big)^{-1},$$

where $\mathfrak{a}$ runs over all integral ideals of K, $\mathfrak{p}$ over all prime ideals of K, and where $N(\mathfrak{a})$ is the absolute norm from K to $\mathbb{Q}$.

This is a generalization of $\zeta(s)$ with similar good properties.

ZETA AND L-FUNCTIONS, II [13]

Theorem 1.1 (Hecke 1920).

(i) The Dedekind zeta function is meromorphic of order 1 *with a simple pole at* $s=1$ *with residue* $2^{r_1}(2\pi)^{r_2}Rh/(w\sqrt{|\Delta(K)|})$*, where* r_1 *is the number of real embeddings of* K*,* r_2 *is the number of pairs of complex embeddings of* K*,* w *is the order of the group of roots of unity in* K*,* R *is the regulator of* K*,* h *is the class number and* $\Delta(K)$ *the discriminant of* K*.*

(ii) We have a functional equation:

$$|\Delta(K)|^{s/2}\left(\pi^{-s/2}\Gamma(s/2)\right)^{r_1}\left((2\pi)^{-s}\Gamma(s)\right)^{r_2}\zeta_K(s)$$

which remains invariant by the change of variable $s\mapsto 1-s$*.*

HECKE CHARACTERS [13]

Absolute values. For each place v, let $\|x\|_v$ be the associated absolute value:

$$\|x\|_v=\begin{cases} N(\mathfrak{p})^{-\operatorname{ord}_{\mathfrak{p}}(x)} & \text{if } v=\mathfrak{p},\\ |x| & \text{if } v=\mathbb{R},\\ |x|^2 & \text{if } v=\mathbb{C}.\end{cases}$$

Ideles. The idele group J is $J=\prod_v K_v^\times$, with the product restricted to elements x with almost every factor $\|x_v\|_v=1$, together with a suitable topology. Note that $K^\times\subset J$ *via* the diagonal embedding.

Hecke Grössencharacter. A continuous homomorphism $\psi: K^\times\backslash J\to\mathbb{T}$.

HECKE CHARACTERS, II [13]

The conductor. A place v is *unramified* for ψ if

$$\psi_v(x_v):=\psi((1,...,1,x_v,1,...))=1$$

whenever $\|x_v\|=1$. The conductor $\mathfrak{f}$ of ψ is the ideal

$$\mathfrak{f}=\prod_{\mathfrak{p}\text{ ramified}}\mathfrak{p}^{m_v}\ ,$$

where m_v is the smallest exponent for which $\psi_v(x_v)=1$ for $x_v\in 1+\mathfrak{p}^{m_v}$.

Grössencharacter of an ideal. It suffices to define it on prime ideals, as $\psi(\mathfrak{p})=\psi(\varpi_v)$ with ϖ_v a uniformizer of $\mathfrak{p}$ if $\mathfrak{p}\nmid\mathfrak{f}$, and 0 otherwise.

HECKE L-FUNCTIONS [13]

For $K_v = \mathbb{R}$ or $\mathbb{C}$, we have

$$\psi_v(x_v) = \left(\frac{x_v}{|x_v|}\right)^{m_v} |x_v|^{i\tau_v} ,$$

where $m_v = 0$ or 1 if $K_v = \mathbb{R}$ and $m_v \in \mathbb{Z}$ if $K_v = \mathbb{C}$.

Theorem 1.2 (Hecke 1920).

(i) The L-function

$$L(s,\psi) = \sum_{\mathfrak{a}} \frac{\psi(\mathfrak{a})}{N(\mathfrak{a})^s} = \prod_{\mathfrak{p}\ \textit{unramified}} \left(1 - \frac{\psi(\mathfrak{p})}{N(\mathfrak{p})^s}\right)^{-1}$$

attached to a non-trivial Grössencharacter ψ is entire of order 1.

(ii) Let $\Delta_\psi = |\Delta(K)|\, N(\mathfrak{f}_\psi)$ and define

$$\Lambda(s,\psi) = (\Delta_\psi)^{s/2} \prod_{K_v=\mathbb{R}} \pi^{-s/2}\Gamma\left(\tfrac{s}{2} + c_v\right) \prod_{K_v=\mathbb{C}} (2\pi)^{-s}\Gamma(s + c_v)\, L(s,\psi) ,$$

where $c_v = (i\tau_v + |m_v|)/2$. Then

$$\Lambda(s,\psi) = w(\psi)\Lambda(1-s,\overline{\psi}) ,$$

for some complex number $w(\psi)$ with $|w(\psi)| = 1$.

ARTIN L-FUNCTIONS [13]

L/K is a Galois extension of degree d of K with Galois group G. Let $\pi : G \to GL_n(\mathbb{C})$ be a representation of G.

The lift $\mathfrak{p}\,\mathcal{O}_L$ to L of a prime ideal $\mathfrak{p}$ of K factors as

$$\mathfrak{p}\,\mathcal{O}_L = \prod_{i=1}^{r} \mathfrak{P}_i^e .$$

e is the ramification index, $|\mathcal{O}_L/\mathfrak{P}_i| = |\mathcal{O}_K/\mathfrak{p}|^f$ and $efr = d$.

G acts on $\{\mathfrak{P}_1,\ldots,\mathfrak{P}_r\}$ by permutations; the subgroup $G_{\mathfrak{P}}$ fixing $\mathfrak{P}$ is the *decomposition group* of $\mathfrak{P}$. The elements $\sigma \in G_{\mathfrak{P}}$ with

$$\sigma x \equiv x^{N(\mathfrak{p})} \pmod{\mathfrak{P}}$$

form a right and left coset $(\mathfrak{P}, L/K)$ (the *Frobenius substitution*) of the *inertia group* $I_{\mathfrak{P}}$ fixing $K(\mathfrak{P}) = O_L/\mathfrak{P}$. Changing $\mathfrak{P}$ into $\eta\mathfrak{P}$ yields $(\eta\mathfrak{P}, L/K) = \eta(\mathfrak{P}, L/K)\eta^{-1}$.

ARTIN L-FUNCTIONS, II [13]

Let $\chi = \mathrm{Tr}(\pi)$ be the character of π and define for $\sigma \in (\mathfrak{P}, L/K)$:

$$\chi(\mathfrak{p}^m) = |I_\mathfrak{p}|^{-1} \sum_{\tau \in I_\mathfrak{p}} \chi(\sigma^m \tau) .$$

Then $\chi(\mathfrak{p}^m)$ is independent of the choices of $\mathfrak{P}$ and σ.

The local L-function.

$$L_\mathfrak{p}(s, \chi, L/K) := \exp\Big(\sum_{m=1}^{\infty} \frac{1}{m} \chi(\mathfrak{p}^m) N(\mathfrak{p})^{-ms} \Big) .$$

The Artin L-function.

$$L(s, \chi, L/K) = \prod_\mathfrak{p} L_\mathfrak{p}(s, \chi, L/K) .$$

THE ARTIN FORMALISM [13]

$L(s, 1, L/K) = \zeta(s, K)$.

Direct sum.

$$L(s, \chi_1 + \chi_2, L/K) = L(s, \chi_1, L/K)\, L(s, \chi_2, L/K) .$$

Restriction. Let $L' \supset L \supset K$ be Galois extensions. Then

$$L(s, \chi, L'/K) = L(s, \chi, L/K) .$$

Induction. Let $L' \supset L \supset K$ be Galois extensions and let χ^* be the character of $G = \mathrm{Gal}(L'/K)$ induced by a character χ of $H = \mathrm{Gal}(L'/L)$. Then

$$L(s, \chi, L'/L) = L(s, \chi^*, L'/K) .$$

The character χ^* is the unique character such that $(\chi^*, \psi)_G = (\chi, \psi|_H)_H$ where $(\ ,\ )_G$ is the scalar product on central functions on G normalized with $(1, 1)_G = 1$.

ARTIN L-FUNCTIONS, III

Theorem 1.3 (Artin 1923). *We have*

$$L(s, \chi, L/K) = \prod_\mathfrak{p} \det \left[I - \frac{\pi(\mathfrak{p})}{N(\mathfrak{p})^s} \right]^{-1} ,$$

where

$$\pi(\mathfrak{p}) = \pi(\sigma) |I_\mathfrak{p}|^{-1} \sum_{\tau \in I_\mathfrak{p}} \pi(\tau) .$$

For the proof, note that $|I_\mathfrak{p}|^{-1} \sum_{\tau \in I_\mathfrak{p}} \pi(\tau)$ is an idempotent.

AN EXAMPLE

$G = \{\pm 1\}$, $L/K = \mathbb{Q}(\sqrt{D})/\mathbb{Q}$, D squarefree. $\Delta = D$ if $D \equiv 1 \pmod 4$, otherwise $\Delta = 4D$.

Case 1: $p \nmid \Delta$, $(p) = \mathfrak{p}\overline{\mathfrak{p}}$. Here $G_{\mathfrak{p}} = \{1\}$ and $(\mathfrak{p}, G) = (\overline{\mathfrak{p}}, G) = 1$ by Fermat's Little Theorem.

Case 2: $p \nmid \Delta$, (p) prime. Here $G_{\mathfrak{p}} = \{\pm 1\}$, $I_{\mathfrak{p}} = \{1\}$ and $((p), G) = -1$, because if (p) does not split then D is not a quadratic residue $\pmod p$.

Case 3: $p \mid \Delta$, $(p) = \mathfrak{p}^2$. Here $G_{\mathfrak{p}} = \{\pm 1\}$, $I_{\mathfrak{p}} = \{\pm 1\}$ and $(\mathfrak{p}, G) = \{\pm 1\}$.

AN EXAMPLE, II

Take π to be the regular representation

$$\pi\{1, -1\} = \left\{ \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right\}.$$

The local factors are:

$$\det \begin{bmatrix} 1 - p^{-s} & 0 \\ 0 & 1 - p^{-s} \end{bmatrix} = (1 - p^{-s})^2 \qquad \text{if } p \text{ splits;}$$

$$\det \begin{bmatrix} 1 & -p^{-s} \\ -p^{-s} & 1 \end{bmatrix} = 1 - p^{-2s} \qquad \text{if } p \text{ remains prime;}$$

$$\det \begin{bmatrix} 1 - \frac{1}{2}p^{-s} & -\frac{1}{2}p^{-s} \\ -\frac{1}{2}p^{-s} & 1 - \frac{1}{2}p^{-s} \end{bmatrix} = 1 - p^{-s} \qquad \text{if } p \text{ ramifies.}$$

Then $L(s, \pi, L/K) = \zeta(s) L(s, (\frac{\Delta}{\cdot}))$.

AN EXAMPLE, III

Identifying $L(s, \pi, L/K) = \zeta(s) L(s, (\frac{\Delta}{\cdot}))$ (where $(\frac{\Delta}{\cdot})$ is the Kronecker symbol) with $\zeta(s, L/K) = \zeta(s) L(s, \chi_{\Delta})$, where now χ_{Δ} is the Dirichlet character, is the quadratic reciprocity law. In the general case of abelian extensions L/K, the corresponding result is Artin's reciprocity law of class field theory. For example, it implies as a special case the famous Kronecker–Weber theorem that every abelian extension of $\mathbb{Q}$ is a subfield of a cyclotomic field.

ARTIN L-FUNCTIONS, IV

Artin's Conjecture. *The L-function $L(s, \chi_\pi, L/K)$ associated to a non-trivial irreducible representation π of* $\mathrm{Gal}(L/K)$ *is an entire function of s of order* 1*.*

Known only in special cases. For G abelian, Artin. Also known for characters expressible as linear combinations with *positive* coefficients of characters induced by cyclic subroups of G. For $\dim(\pi) = 2$ and $G = S_3$ and $G = S_4$, Langlands [15], Tunnell [22]. For $G = A_5$ with some conditions, Taylor [20], Shepherd-Barron & Taylor [18], Buzzard & Dickinson & Shepherd-Barron & Taylor [2], Buzzard & Stein [3].

Brauer's Theorem. *$L(s, \chi_\pi, L/K)$ is meromorphic of order 1 and satisfies a functional equation ($\Lambda = L \times \{\Gamma$-factors$\}$)*

$$\Lambda(s, \chi_\pi, L/K) = w(\chi_\pi, L/K)\Lambda(1-s, \widetilde{\chi}_\pi, L/K) ,$$

where $\widetilde{\chi}_\pi$ is the character of the contragredient of π.

SOME MODULAR FORMS

Let $f(z)$ be a holomorphic modular form of weight k for a subgroup $\Gamma < \Gamma(1)$ generated by $z \mapsto z + h$ and $z \mapsto -1/z$:

$$f(\gamma z) = \varepsilon(\gamma)(cz+d)^k f(z) , \qquad \gamma = \begin{bmatrix} a & b \\ c & d \end{bmatrix} ,$$

with $\varepsilon(\gamma)$ an appropriate set of multipliers (*Nebentypus*).

Then $f(z)$ is periodic and has a Fourier expansion

$$f(z) = \sum_{n=0}^{\infty} a_n \mathrm{e}^{2\pi \mathrm{i} z/h} .$$

By the Mellin transform, $L(s, f) = \sum_{n=1}^{\infty} a_n n^{-s}$ is meromorphic of order 1, with a simple pole at $s = k$ if $a_0 \neq 0$, and

$$(2\pi/h)^{-s}\Gamma(s)L(s,f) = w\,(2\pi/h)^{s-k}\Gamma(k-s)L(k-s,f) ,$$

for $w = \mathrm{i}^k \varepsilon([z \mapsto -1/z])$.

A CONVERSE THEOREM

Theorem 1.4 (Hecke 1936). *Conversely, given $L(s, f)$ with the above properties one recovers a modular form f of weight k for Γ, by setting $a_0 = \mathrm{i}^{-k} w$ in case $L(s, f)$ has a pole at $s = k$.*

Example. Take $h = 2$ and

$$\theta(z) = \frac{1}{2} \sum_{n=-\infty}^{\infty} \mathrm{e}^{\pi \mathrm{i} n^2 z} .$$

Then $\theta(z)$ is a modular form of weight 1/2, multiplier 1 and $L(s, \theta) = \zeta(2s)$. The space of such forms for Γ has dimension 1, hence $\zeta(2s)$ is the unique (up to a scalar) Dirichlet series satisfying the same functional equation as $\zeta(2s)$.

A CONVERSE THEOREM, II [25]

Hecke's converse result uses only the cusp at $i\infty$. Weil's new idea: Control of the Fourier expansions at every cusp by 'twisting' the Dirichlet series with Dirichlet characters.

Theorem 1.5 (Weil 1967). *Let $L(s,f)=\sum a_n n^{-s}$ and write, for a Dirichlet character $\chi \pmod r$:*

$$\Lambda(s,f\otimes\chi)=(2\pi)^{-s}\Gamma(s)\sum_{n=1}^{\infty}a_n\chi(n)n^{-s}\ .$$

Suppose there are N, k such that for every primitive $\chi \pmod r$ with $(r,N)=1$ we have that $\Lambda(s,f\otimes\chi)$ is entire of order 1 and

$$\Lambda(s,f\otimes\chi)=w_\chi r^{-1}(r^2N)^{k/2-s}\Lambda(k-s,f\otimes\overline{\chi})$$

with $w_\chi=\mathrm{i}^k\chi(N)G(\chi)^2$ and $G(\chi)=\sum_{n \pmod r}\chi(n)\exp(2\pi\mathrm{i}n/r)$.

Then $L(s)=L(s,f)$ with f a holomorphic cusp form for $\Gamma_0(N)$.

THE HASSE–WEIL ZETA FUNCTION

The Hasse–Weil zeta function. Let V/K be a variety over a number field. Then for all except finitely many prime ideals $\mathfrak{p}$ the reduction $\overline{V}_\mathfrak{p}$ is defined over the finite field $\mathcal{O}_K/\mathfrak{p}$ and yields a Zeta function $Z(T,\overline{V}_\mathfrak{p})$. The global zeta function of V is now

$$\prod_{\mathfrak{p}}Z(N(\mathfrak{p})^{-s},\overline{V}_\mathfrak{p})\ ,$$

where the product runs over all prime ideal where the reduction is defined.

If V'/K is another model of V the zeta functions are the same up to finitely many factors.

A difficulty. Define 'good factors' even at places of bad reduction and 'good models' for which the zeta function behaves nicely.

SOME EXAMPLES

Example. Let V be the projective space $\mathbb{P}^n/\mathcal{O}_K$. Then

$$\zeta(s,V)=\zeta_K(s)\zeta_K(s-1)\cdots\zeta_K(s-n)\ .$$

Example (Deuring, 1953–57). Let E be an elliptic curve over a number field L, with complex multiplication in the imaginary quadratic field $K=\mathrm{End}(E)\otimes\mathbb{Q}$. Assume $K\subset L$. Then there is a model of E/L and a Hecke Grössencharacter ψ of L such that

$$\zeta(s,E)=\zeta_L(s)\zeta_L(s-1)L(s-1/2,\psi)L(s-1/2,\overline{\psi})\ .$$

Example (Taniyama, 1957). The previous example extends to abelian varieties of CM type.

THE TANIYAMA CONJECTURE

Eichler (1953) proved the functional equation for zeta functions of modular curves $X_0(N) = \mathcal{H}/\Gamma_0(N)$ of genus 1, by showing that in this case $L(s, X_0(N))$ was the Mellin transform of a cusp form of weight 2. Shimura [19] extended this to certain other cases. On the basis of this evidence, Taniyama suggested this held in general.

Conjecture 1.6 (Taniyama 1955, Shimura, Weil, . . .). *Every elliptic curve over $\mathbb{Q}$ is uniformized by a cusp form of weight 2 for $\Gamma_0(N)$. Equivalently, every elliptic curve $E/\mathbb{Q}$ admits the modular curve $X_0(N)$ as a ramified covering, for some N.*

Proved by Wiles [26], Wiles & Taylor [21], in the semistable case (namely multiplicative bad reduction only) and now in general by Breuil & Conrad & Diamond & Taylor [1].

FIBONACCI AND CONGRUENT NUMBERS [8]

Fibonacci

Fibonacci sequence

$$1, 1, 2, 3, 5, 8, \ldots; \quad f_{n+1} = f_n + f_{n-1}$$

The *Liber Quadratorum*

Fibonacci's formula

$$(a^2 + b^2)(c^2 + d^2) = (ad \pm bc)^2 + (ac \mp bd)^2$$

Congruent numbers m

$$h^2 + m = \square, \quad h^2 - m = \square$$

$$h^2 = a^2 + b^2, \quad m = 2ab = 4 \times area$$

Fibonacci: $m \neq \square$

The congruent number 157

The smallest solution is (Zagier)

$$a = \frac{3401649243913217525608770}{411340519227716149383203},$$

$$b = \frac{411340519227716149383203}{43333111387429522619220}.$$

CONGRUENT NUMBERS, II [23]

The solution? (Tunnell 1983). *Let $g = q\prod(1 - q^{8n})(1 - q^{16n})$, $\theta_2 = \sum q^{2n^2}$, $\theta_4 = \sum q^{4n^2}$, $q = \mathrm{e}^{\pi \mathrm{i} z}$, and define cusp forms of weight $3/2$ for $\Gamma_0(32)$:*

$$g\theta_2 = \sum a(n)q^n , \qquad g\theta_4 = \sum b(n)q^n .$$

Then a squarefree m is not a congruent number if $a(m) \neq 0$ (m odd), and if $b(m/2) \neq 0$ (m even). The converse is true if the B & S-D conjecture holds for $y^2 = x^3 - m^2x$ (or $my^2 = x^3 - x$).

Comments on proof: m is congruent if and only if the curve E_m defined by $my^2 = x^3 - x$ has rational solutions with $y \neq 0$. The connection with cusp forms uses a deep result of Waldspurger for computing $L(1, E_m)$ (for example, for odd m it yields $L(1, E_m) = \beta a(m)^2/(4\sqrt{m})$, $\beta = \int_1^\infty (x^3 - x)^{-1/3} \mathrm{d}x = 2.62205\ldots$), theta lifts and the B&S-D conjecture.

THE NEW ROSETTA STONE

The intertwining of geometry, automorphic theory, and L-functions, was compared by André Weil with the reading of a Rosetta stone for mathematics.

Motivic writing. L-functions can be defined from geometry (Hasse, Weil, ...)

Galois writing. L-functions can be defined from finite dimensional representations of the absolute Galois group $\mathrm{Gal}(\overline{K}/K)$ acting on a vector space V (Artin, Weil, Serre, ...)

Automorphic writing. L-functions can be defined globally from automorphic forms on algebraic groups modulo discrete subgroups (Hecke, Langlands, ...)

AUTOMORPHIC *L*-FUNCTIONS [16]

Langlands $\sim$ 1970. Vastly extended the concept of automorphic form and automorphic L-function.

Remark. A Hecke character is nothing else than a representation of $GL_1(\mathbb{A})$ in the space of continuous functions on $GL_1(K)\backslash GL_1(\mathbb{A})$.

An automorphic representation is an irreducible component π of a representation of the group $GL_n(\mathbb{A})$ on the space of continuous functions on $GL_n(K)\backslash GL_n(\mathbb{A})$ (with technical conditions). One can then attach to π an L-function, with functional equation $L(s,\pi) = w(\pi)L(1-s,\widetilde{\pi})$ with $\widetilde{\pi}$ the contragredient. Also π decomposes as a tensor product $\otimes\pi_v$ of local components, yielding an Euler product for $L(s,\pi)$ with standard factors of degree n.

AUTOMORPHIC *L*-FUNCTIONS, II [16]

Automorphic L-functions (Langlands [14]). A concept which fuses together the Artin and Hecke concepts. Given a connected reductive group G/K and a finite extension L/K, one considers an extension ${}^LG$ of G by $\mathrm{Gal}(L/K)$, a finite dimensional complex representation ρ of ${}^LG$, and a representation π of $G(\mathbb{A})$. The theory of Hecke operators gives us, for each local factor π_v of π, a conjugacy class $g_v = g(\pi_v) \in {}^LG$ which generalizes the notion of Frobenius substitution.

The automorphic L-function associated to ρ and π is a product of local factors where for almost every v one has

$$L_v(s, \pi_v, \rho) = \det\left(I - \rho(g_v)N(\mathfrak{p})^{-s}\right)^{-1} .$$

AUTOMORPHIC *L*-FUNCTIONS, III [16]

The goal. The reciprocity law, namely: *Given ρ and π there is π' of $G(\mathbb{A})$ such that $L_v(s, \pi_v, \rho) = L_v(s, \pi'_v)$ for almost every v and $L(s, \pi, \rho) = L(s, \pi')$.*

The first tool. The *principle of functoriality.* If H and G are two reductive groups and ${}^LG \to \mathrm{Gal}(L/K)$ factors as

$${}^LG \xrightarrow{\varphi} {}^LH \to \mathrm{Gal}(L/K) ,$$

then one expects for each π for G to attach Π for H such that one has the equality of conjugacy classes $\{g(\Pi_v)\} = \{\varphi(g(\pi_v))\}$ for almost every v. An important special case is *base change* [15], known in some cases.

Others tools. Converse theorems (Cogdell and Piatetski-Shapiro [4]), theta-liftings, the Selberg–Arthur trace formula.

READING THE ROSETTA STONE

Automorphic = Galois. This is a key step with very deep implications. For GL_1, it is Artin's abelian reciprocity law of class field theory, a vast generalization of the quadratic reciprocity law. For GL_2 it is known for dihedral (reduces to GL_1), tetrahedral and octahedral representations and many (but not yet all) icosahedral representations, i.e. $G = S_3, S_4, A_5$ ([15], [23], [20], [18], [2], [3]).

Galois = Motivic. This is also a key step, understood in very few cases, namely GL_1 (Artin, Hecke), elliptic curves $E/\mathbb{Q}$ (the Taniyama conjecture).

Motivic = Automorphic. Known in very few cases. Possibly there are more automorphic L-functions than motivic L-functions coming from geometry.

APPLICATIONS

If

$$L(s,f) = \prod_v \left(1-\omega_1(\mathfrak{p})N(\mathfrak{p})^{-s}\right)^{-1}\left(1-\omega_2(\mathfrak{p})N(\mathfrak{p})^{-s}\right)^{-1}$$

the symmetric k-th power is

$$L(s, \mathrm{Sym}^k f) = \prod_v \prod_{j=0}^{k} \left(1-\omega_1(\mathfrak{p})^j \omega_2^{k-j}(\mathfrak{p})N(\mathfrak{p})^{-s}\right)^{-1} .$$

A deep conjecture is that these symmetric powers have analytic continuation and functional equation. A success of these methods has been to prove such a conjecture for $k = 2, 3, 4$ ($k = 2$ by Rankin and Selberg for classical cusp forms, Gelbart and Jacquet [7] in general, $k = 3$ and 4 by Kim and Shahidi [11]).

CLASSICAL PROBLEMS

We have a good formal understanding for L-functions for Dirichlet characters and cusp forms for congruence subgroups of $\Gamma(1)$, but only limited information on analytical behavior. The functional equation has the form $\Lambda(s,f) = w(f)\Lambda(k-s,\overline{f})$, $k = 1$ or 2. An Euler product for $L(s,f)$ has local factors given by polynomials of degree k. The integer k is the *degree* of $L(s,f)$.

The Generalized Riemann Hypothesis (GRH). *The zeros of the functions $\Lambda(s,f)$ with Euler product all lie on the vertical line at the center $k/2$ of the critical strip (the critical line).*

The Generalized Lindelöf Hypothesis (GLH). *For every fixed $\varepsilon > 0$, $L(s,f)$ has order $N^\varepsilon(|s|+1)^\varepsilon$ in the half-plane to the right of the critical line (except at a possible pole). Here N is the conductor.*

CLASSICAL PROBLEMS, II

Let $\mu(\sigma,f)$ be defined as the best exponent for which

$$|L(\sigma+\mathrm{i}t,f)| \ll \left(N(|t|+1)\right)^{\mu(\sigma,f)+\varepsilon} .$$

Then the functional equation and convexity yields $\mu(\sigma,f) \le (k-\sigma)/2$ for $0 \le \sigma \le k$. The Lindelöf hypothesis is $\mu(\sigma,f) = 0$ for $k/2 \le \sigma \le k$; a *subconvexity bound* is the statement $\mu(\sigma) < (k-\sigma)/2$ for $k/2 \le \sigma \le k$. Such a statement has deep arithmetic consequences which are unattainable using the convexity bound alone. The estimate in the conductor is particularly hard (Duke & Friedlander & Iwaniec [5], [6]).

CLASSICAL PROBLEMS, III

The Generalized Ramanujan Conjecture (GRC). Ramanujan conjectured, on the basis of numerical evidence, that $|\tau(p)| \le 2p^{11/2}$ for every prime p. In general, this is about the coefficients a_n in $L(s,f) = \sum a_n n^{-s}$. Then GRC is the statement

$$|a_n| \ll n^{(k-1)/2+\varepsilon} ,$$

for every fixed $\varepsilon > 0$.

GRC is a deep statement. For $K = \mathbb{Q}$ and $k = 2$, it is known when f is a holomorphic cusp form of even integral weight for $\Gamma(1)$, as a consequence of Deligne's GRH for varieties over finite fields (1974). It is open already for f a non-holomorphic cusp form (Maaß wave form) for $\Gamma(1)$.

FAMILIES

Let $\{\lambda_j\}$ be a real sequence, $\lambda_j \sim j$. Consider the gaps $\Delta_j = \lambda_{j+1} - \lambda_j$ and set

$$\mu_1(N)[a,b] = \frac{1}{N}\#\{j : \Delta_j \in [a,b]\} , \quad 0 \le j < N .$$

Quite often one finds a Cauchy–Poisson distribution

$$\mu_1(N) \to \mathrm{e}^{-x}\mathrm{d}x .$$

Example. This is expected for the sequence $\{p_j/\log p_j\}$, although it remains hopeless to prove.

Example. Again, expected for the (ordered) sequence $\{\pi 2^{-9/4}(m^2 + \sqrt{2}n^2)\}$ and, again, completely open.

Problem. What is the expected behavior for $\{1/(2\pi)\,\gamma\log\gamma\}$, where $\zeta(1/2 + \mathrm{i}\gamma) = 0$ and $\gamma > 0$? (There are applications.)

FAMILIES, II [9]

For $A \in U(N)$, consider the eigenvalues $z_1, \dots, z_N$ on the unit circle ordered by increasing argument (mod 2π). Let

$$\mu_{k,N}(A)[a,b] = \frac{1}{N}\#\Big\{j : \frac{N}{2\pi}\arg(z_{j+k}/z_j) \in [a,b]\Big\} .$$

Theorem 1.7 (Gaudin 1961, Katz & Sarnak 1999).

$$\int_{U(N)} \mu_{k,N}(A)\mathrm{d}A \to \mu_k([a,b]) ,$$

(here dA *is the normalized Haar measure) with*

$$\mathrm{d}\mu_k = \frac{\mathrm{d}^2}{\mathrm{d}s^2}\left(\sum_{j=0}^{k-1} \frac{k-j}{j!}\left(\frac{\partial}{\partial T}\right)^j \det\big(I + TK(s)\big)\big|_{T=1}\right)\mathrm{d}s$$

and $K(s)$ the operator defined by

$$K(s)\phi(x) = \int_{-s/2}^{s/2} \frac{\sin(x-y)}{\pi(x-y)}\phi(y)\mathrm{d}y\ .$$

Conjecture 1.8 (Montgomery, Katz & Sarnak). *The sequence of zeros of $\zeta(s)$ satisfies the above $U(N)$ statistics for eigenvalues of random unitary matrices.*

FAMILIES, III

Extensive calculation by Odlyzko [17] with zeros of $\zeta(s)$ around 10^{20} show a total agreement with the prediction. The only problem is: Why is this so?

There are similar formulas for the other classical groups $SU(N)$, $O(N)$, $SO(N)$, $USp(N)$. The amazing thing is that certain families of L functions seem to follow the same correlations. For example, the distribution of the j-th zero of $L(s,\chi)$, χ a primitive quadratic character, follows the USp prediction. Instead, the j-th zero of $L(s, E\otimes\chi)$, E an elliptic curve, follows the O prediction (two cases, according to the sign $\pm$ in the functional equation, corresponding to the two connected components $O^{\pm}$ of O). There is numerical evidence that these are the true statistics and some consequences of them, pertaining to the behaviour of moments of small order of L-functions on the critical line, have also been verified unconditionally.

FAMILIES, IV

Katz and Sarnak have shown that in the function field analogue the prediction are verified for families for which Deligne's theory applies, and the associated groups are nothing else than the monodromy groups of the families.

Question. For families of classical L-functions, what should replace monodromy so as to explain how these laws arise?

Question. Is this phenomenon peculiar to L-functions or is it instead the expression of a '*universality law*' which holds in a much wider context?

Question. Is there a way of formulating a program to prove GRH following Deligne's blueprint in this new context?

FAMILIES, V

The predictions on correlations have changed our way of thinking about L-functions.

Example. Until very recently, most analytic number theorists thought that the maximum order of magnitude of $\log^+|\zeta(1/2+\mathrm{i}t)|$ was $\sqrt{\log|t|\,\log\log|t|}$, based on the known Gaussian behavior of $\log|\zeta(1/2+\mathrm{i}t)|/\sqrt{\pi\log\log|t|}$ and a probabilistic extrapolation. On RH, it was known that this maximum order cannot exceed $\log|t|/\log\log|t|$, but this is only an upper bound and the gap between the two was ascribed to an intrinsic 'weakness' of analytic methods.

Today, the work of Keating and Snaith [10] leads us to believe that the true maximum order of $\log^+|\zeta(1/2+\mathrm{i}t)|$ is $\log|t|/\log\log|t|$. This came as a total surprise to experts.

FAMILIES, VI

In the function field case, the discovery by Ulmer [24] of elliptic curves over $\mathbb{F}_p$ with rank as big as $\log N/\log\log N$ (N is the conductor) confirms, *via* a Birch & Swinnerton–Dyer conjecture, the new prediction that the maximum order of $\log^+|\zeta(1/2+\mathrm{i}t)|$ is $O(\log|t|/\log\log|t|)$.

Conclusion. The analogy with the function field case is often a good predictor for the classical case too.

Conclusion. The recent proof by Lafforgue [12] in the function field case that **motivic = automorphic** gives support to the hoped deciphering of the new Rosetta stone, namely that **motivic = automorphic** also holds in the classical case.

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New Encounters in Combinatorial Number Theory: From the Kakeya Problem to Cryptography

J. Bourgain

Institute for Advanced Study, School of Mathematics, Princeton, NJ 08540, USA
bourgain@math.ias.edu

1 Basic Definitions and Previous Results

A Kakeya set in $\mathbb{R}^d$ is a Borel measurable set $S \subset \mathbb{R}^d$ $(d \geq 2)$ containing a line segment in every direction.

Conjecture 1.1. If $S \subset \mathbb{R}^d$ is a Kakeya set, then $\dim S = d$ ('dim' denotes Hausdorff dimension).

Such sets may be of zero Lebesgue measure (construction for $d = 2$ due to Besicovitch [1]).

The conjecture has been verified for $d = 2$ (see [15]) but it remains open for $d = 3$. In the case $d = 3$, $\dim S \geq 5/2$ (see [29]) and this is essentially the best result to date. In general, $\dim S \geq d/2 + 1$.

This problem has relevance to various issues in Harmonic Analysis involving curvature, such as

- the disproof of the ball multiplier conjecture [19]
- bounds on oscillatory integrals, see in particular [3].
- E. Stein's restriction conjecture [26]:

  Let $\mu \in M(S^2)$ such that $\|\frac{\mathrm{d}\mu}{\mathrm{d}\sigma}\|_\infty < \infty$. Then $\hat{\mu} \in L^p(\mathbb{R}^3)$ for all $p > 3$.

The first improvements beyond the Stein–Tomas estimate $\|\hat{\mu}\|_4 \leq C\|\frac{\mathrm{d}\mu}{\mathrm{d}\sigma}\|_2$ appears in [2] where the problem is also linked to the above Conjecture. The best result to date is due to T. Tao [27], namely $\|\hat{\mu}\|_p \leq C\|\frac{\mathrm{d}\mu}{\mathrm{d}\sigma}\|_\infty$ for $p > 10/3$.

1.1 Relevance to the Distribution of Dirichlet Sums (Montgomery's Conjectures)

These conjectures originate from density problems (such as the density conjecture) for the zeros of the ζ–function and Dirichlet L–functions. A detailed presentation of the interrelation between these different topics may be found in [31] and [4]. Those survey papers of course do not cover more recent developments.

2 Recent Developments

There are several new connections with Combinatorics and Combinatorial Number Theory.

2.1 Connections with Combinatorics

Theorem 2.1 (Wolff [30]). *Let $A \subset \mathbb{R}^2$ be a Borel measurable set containing a circle of arbitrary radius $\rho \in [1, 2]$. Then* $\dim A = 2$.

The proof is based on methods from computational geometry (the cell decomposition technique), see [13].

2.2 Connections with Combinatorial Number Theory

Key results involved in the link with Combinatorial Number Theory were provided by

- Freiman (structure of sets with 'small' sum-sets)
- Plunnecke (sum-sets inequalities)
- Rusza (-, new proof of Freiman's theorem)
- Gowers (new proof of the Balog–Szemeredi theorem)

In this spirit significant improvements are obtained in large dimension ($d \geq 5$) using methods from Additive Number Theory. For example

Theorem 2.2 ([22]). *If S is a Kakeya set in $\mathbb{R}^d$ then*

$$\dim S \geq (2 - \sqrt{2})(d - 4) + 3 \, .$$

The Kakeya problem turns out to be embedded in a class of questions from combinatorial number theory, often with a large gap between what is likely to be true and what may be proven with the present knowledge. There are many partial but few final results.

3 Geometric and Algebraic Counterparts

There has been no significant numerical progress in $d = 3$ beyond $5/2$. Problems appear already on purely *geometric* or *algebraic* level (without metrical structure).

3.1 Geometric Setting

Let $S \subset \mathbb{R}^3$ be a finite set and $\mathcal{L}$ a collection of N^2 lines such that no plane in $\mathbb{R}^3$ contains more than N lines from $\mathcal{L}$. Assume that for each $\ell \in \mathcal{L}$

$$|\ell \cap S| \geq N .$$

Is it then true that

$$|S| \gg N^{3-\varepsilon} \ ?$$

Remark 3.1. The Szemeredi–Trotter theorem implies that

$$|S|^2 > cN^2 N^3 \quad \Rightarrow \quad |S| > cN^{5/2}$$

(using only that $\mathcal{L}$ consists of distinct lines).

Small improvement known: $|S| > N^{5/2+\delta}$.

3.2 Algebraic Setting

Let $S \subset \mathbb{F}_p^3$ (p prime) contain a line in every direction. Is it true that

$$|S| \gg p^{3-\varepsilon} \ ?$$

It is known (see [12]) that

$$|S| > p^{5/2+\delta} .$$

4 The Relation with Sum-product Problems

This development originates from [23].

It appears that the Kakeya (and related) conjectures require a better understanding of purely one-dimensional issues, basically expressing that either the sum or the product set of a given set A is significantly larger than A itself. This 'principle' has dimensional, arithmetical and metrical appearances.

4.1 Erdös–Volkman Ring Problem, 1966

Let S be a Borel subring of $\mathbb{R}$ ($x, y \in S \Rightarrow x + y, x \cdot y \in S$). Then

$$\dim S = 0 \quad \text{or} \quad \dim S = 1 .$$

This problem was solved by Edgar–Miller [18] and independently by the author [7].

4.2 The Erdös–Szemeredi Sum-product Problem, 1986

Let A be a finite subset of $\mathbb{Z}$ (or $\mathbb{R}$). Then is it true that

$$|A+A| + |A\cdot A| \gg |A|^{2-\varepsilon} \ ?$$

This problem is still open. The best result to date is the following result by J. Solymosi [24]

$$|A+A| + |A\cdot A| > \frac{|A|^{14/11}}{(\log |A|)^3} \ .$$

4.3 The 'Discretized' Ring Problem [23], 2001

Let $A \subset [1,2]$ be a union of δ-intervals and satisfying $(0<\sigma<1)$

(i) $|A| > \delta^{1-\sigma+}$,
(ii) $|A\cap I| < r^\sigma \delta^{1-\sigma}$ for all $\delta < r < 1$ and I an interval of size r.

Is it then true that

$$|A+A| + |A\cdot A| > \delta^{1-\sigma'} \quad \text{for} \quad \sigma'(\sigma) > \sigma \ ?$$

The answer to this problem has been proven to be affirmative (see [7]).

4.4 The Sum-product Problem in $\mathbb{F}_p$ [12], 2003

For every $\varepsilon > 0$ there exists a $\delta > 0$ such that if $A \subset \mathbb{F}_p$ and $p^\varepsilon < |A| < p^{1-\varepsilon}$, then

$$|A+A| + |A\cdot A| > |A|^{1+\delta} \ .$$

The same conclusion holds assuming $|A| < p^{1-\varepsilon}$ (see [11]). The approach to prove this is closely related to the work of Edgar–Miller.

It turns out that besides the lower bound $|S| > p^{5/2+\delta}$, if S is a Kakeya set in $\mathbb{F}_p^3$, the sum-product theorem in $\mathbb{F}_p$ permits us quite substantial progress on issues of bounding various exponential sums (that seem to lie beyond the reach of 'conventional' technology). In the remainder of this exposé, we will review a few recent results obtained by this method.

5 Exponential Sum Estimates

The sum-product theorem in $\mathbb{F}_p$ offers a new approach to exponential sum estimates.

Theorem 5.1 (Bourgain–Konyagin [11]). *Let G be a subgroup of $\mathbb{F}_p^*$ and $|G| > p^\delta$ (p prime, $\delta > 0$ an arbitrary fixed constant). Then*

$$\max_{a\in\mathbb{F}^*}\left|\sum_{x\in G}\exp\left(2\pi\mathrm{i}\frac{ax}{p}\right)\right| \le |G|p^{-\gamma}\ ,$$

where $\gamma = \exp(-C\delta^{-C})$ and C is some constant.

Earlier results have been obtained by Korobov ($\delta > 1/2$), Shparlinski ($\delta > 3/7$), Heath–Brown–Konyagin ($\delta > 1/3$) and finally by Konyagin ($\delta > 1/4$). The latter three approaches were based on Stepanov's method. See [21] for a survey and references.

Corollary 5.2. *If $k < p^{1-\delta}$ then there is an estimate on the Gauss-sum*

$$\max_{a\in\mathbb{F}_p^*}|G_p(a,k)| < p^{1-\delta'} \qquad \delta' = \delta'(\delta) > 0\ ,$$

where

$$G_p(a,k) = \sum_{x=0}^{p-1} e_p(ax^k)\ .$$

Remark 5.3. (i) The classical estimate is $|G_p(a,k)| \le (k, p-1)\sqrt{p}$. This is always nontrivial for $k < p^{1/2-\varepsilon}$.

(ii) In general, if $f(x) \in \mathbb{Z}[x]$ is a polynomial of degree k then

$$\left|\sum_{j=0}^{p-1} e_p\big(f(x)\big)\right| < k\sqrt{p}\ .$$

This is due to A. Weil. Deligne made a generalization to varieties.

In certain cases, Mordell's estimate is better.

There is an improved version (see [16]) stated as follows: Let $f(x) = \sum_{i=1}^r a_i x^{k_i}$, $a_i \in \mathbb{F}_p^*$, $1 \le k_1 < k_2 < \cdots < k_r < p-1$. Then

$$\left|\sum_{x=1}^{p-1} e_p(f(x))\right| \le 4^{1/r}(k_1,\ldots,k_r)^{1/r^2} p^{1-1/2r}\ .$$

See also [17] for the binomial case.

(iii) Corollary 5.2 is previously known for $k < p^{3/4-\varepsilon}$, a result by Konyagin [20].

Theorem 5.4 ([5]). *Let $\theta \in \mathbb{F}_p^*$ be of multiplicative order t and $t \ge t_1 > p^\delta$. Then*

$$\max_{a\in\mathbb{F}^*}\left|\sum_{s=1}^{t_1} e_p(a\theta^s)\right| < t_1 p^{-\delta'} \qquad \delta' = \delta'(\delta) > 0\ .$$

Theorem 5.5 ([5]). *Let $\theta \in \mathbb{F}_p^*$ be of multiplicative order $t > p^\delta$. Then*

$$\max_{(a,c,p)=1} \sum_{s'=1}^{t} \left| \sum_{s=1}^{t} e_p(a\theta^s + c\theta^{ss'}) \right| < t^2 p^{-\delta'} .$$

Corollary 5.6. *Let $\theta \in \mathbb{F}_p^*$ be of multiplicative order $t > p^\delta$. Then*

$$\max_{(a,b,c,p)=1} \left| \sum_{s=1}^{t} \sum_{s'=1}^{t} e_p(a\theta^s + b\theta^{s'} + c\theta^{ss'}) \right| < t^2 p^{-\delta'} .$$

Corollary 5.7. *Let $\theta \in \mathbb{Z}$ be of multiplicative order $t > p^\delta$ modulo p. Then the triples*

$$\left(\left\{ \frac{\theta^x}{p} \right\}, \left\{ \frac{\theta^y}{p} \right\}, \left\{ \frac{\theta^{xy}}{p} \right\} \right)_{x,y=1,\ldots,t}$$

have discrepancy $D < p^{-\delta'}$.

Remark 5.8. (i) Theorem 5.5 and Corollaries 5.6 and 5.7 are previously known for $t > p^{3/4+\varepsilon}$. See in particular the paper [14].

(ii) If we fix $\theta \in \mathbb{Z}$, then the multiplicative order t of θ modulo p satisfies $t > p^{1/2-\varepsilon}$ for almost all primes p.
There are infinitely many primes p such that $p-1$ has a prime divisor $t > p^\alpha, \alpha > 0.677$ (see [10]).

(iii) $(\theta^x, \theta^y, \theta^{xy})$ are the *Diffie–Hellman triples* in cryptography and θ^{xy} is the D-H secret key.
The DHC-assumption: 'there is no polynomial-time algorithm that, given $p, \theta, \theta^x, \theta^y$, computes θ^{xy}'.
More precisely: Let p be an n-bit prime and let $\theta \in \mathbb{F}_p^*$ be of multiplicative order $t > p^\delta$. Then 'the distribution of binary strings that represents $(\theta^x, \theta^y, \theta^{xy})$, where x, y are chosen uniformly in $\mathbb{F}_p^*$, has statistical distance from the uniform distribution that is exponentially small in n'.
This result is established in [14] for $t > p^{3/4+\varepsilon}$.

6 The Method

Assume that $H < \mathbb{F}_p^*$ is a multiplicative subgroup, where $|H| > p^\delta$. Iterating the sum-product theorem, it follows that

$$\forall \varepsilon > 0, \exists k = k(\delta, \varepsilon) \quad \text{such that} \quad |kH| = |\underbrace{H + \cdots + H}_{k}| > p^{1-\varepsilon} .$$

It turns out there is the following stronger property on the decay of convolutions.

Theorem 6.1. *Let H be as above. For all $\varepsilon > 0$, there is a $k = k(\varepsilon, \delta)$ such that denoting*

$$\nu = \frac{1}{|H|} \sum_{x \in H} \delta_x \ ,$$

we have

$$\max_x |\nu^{(k)}(x)| < p^{-1+\varepsilon} \qquad \nu^{(k)} = \underbrace{\nu * \cdots * \nu}_{k} \ .$$

Assuming that H is symmetric (which we may), it follows that

$$p\nu^{(2k)}(0) = \sum_{\xi \in \mathbb{F}_p} |\hat{\nu}(\xi)|^{2k} = \sum_{\xi \in \mathbb{F}_p} |H|^{-2k} \Big| \sum_{x \in H} e_p(x\xi) \Big|^{2k} < p^{\varepsilon} \ .$$

Fix $a \in \mathbb{F}_p^*$. By invariance

$$\sum_{x \in H} e_p(ax) = \sum_{x \in H} e_p(ahx) \ , \qquad \forall h \in H \ ,$$

and from the preceding

$$|H| \Big| \sum_{x \in H} e_p(ax) \Big|^{2k} < |H|^{2k} p^{\varepsilon}$$

$$\Big| \sum_{x \in H} e_p(ax) \Big| < |H| p^{(\varepsilon - \delta)/2k} < p^{-\delta/4k} |H|$$

and Theorem 5.1 follows.

Remark 6.2. (i) The previous Theorem remains valid under weaker assumptions on $H \subset \mathbb{F}_p$. It suffices that $|H| > p^{\delta}$ and H has a small product set, i.e.

$$|H \cdot H| < C|H| \ .$$

As a consequence we obtain Theorem 5.4 by taking

$$H = \{\theta^s \mid s = 1, \ldots, t_1\} \ .$$

(ii) There are versions of the Theorem for subgroups $H \subset \mathbb{F}_p^* \times \mathbb{F}_p^*$ (and more general products). Notice that clearly in $\mathbb{F}_p \times \mathbb{F}_p = R$, there is no sum-product theorem valid without some restrictions. However, the following holds

Theorem 6.3. *Let $H \subset \mathbb{F}_p^* \times \mathbb{F}_p^*$, $|H| > p^{\delta}$ and $|H \cdot H| < C|H|$. Let*

$$\nu = \frac{1}{|H|} \sum_{x \in H \cup (-H)} \delta_x$$

and assume that there is an integer k (bounded) such that

$$|\nu^{(2k)}(0)| < p^{-1-\varepsilon} \ ,$$

for some $\varepsilon > 0$. Then there is a $k_1 = k_1(k, \varepsilon)$ such that

$$|\nu^{(2k_1)}(0)| < p^{-2+\varepsilon} \ .$$

Theorem 5.5 follows by taking $H = H_{s'} = \{(\theta^s, \theta^{s's}) \mid s = 1, \ldots, t\}$.

(iii) The basic philosophy of the Theorem is at least formally reminiscent of results obtained in the 80's by N. Varopoulos (see e.g. [28]) for random walks on finitely generated groups: *growth of balls defined by the word-metric implies transience properties of the random walk.*

7 Some Other Applications

7.1 Uniform Distribution of Mersenne Numbers

The *Mersenne numbers* are defined as $M_q = 2^q - 1$, where q is prime.

Theorem 7.1. *For almost all primes p, the sequence*

$$\left\{ \frac{M_q}{p} \right\}_{q=1,\ldots,t^{2+\varepsilon} q \ prime}$$

is uniformly distributed, t = multiplicative order of 2 modulo p.

The proof is obtained by combining the Vinogradov–Vaughan estimate of $\sum_{n \leq N} \Lambda(n) f(n)$, where $\Lambda(n)$ is the Von Mangoldt function, with Theorems 5.4 and 5.5. This result was established earlier in [9], assuming GRH.

7.2 Prime Divisors of 'Sparse Integers'

For $g \geq 2$ and $s \geq 1$ two integers and $\mathcal{D} = \{d_i\}_{i=0}^{s}$ a sequence of $s+1$ non-zero integers, denote

$$\mathcal{S}_{g,s}(\mathcal{D}) = \{d_0 + d_1 g^{m_1} + \cdots + d_s g^{m_s} \mid m_i \in \mathbb{Z}_+\} \ .$$

Theorem 7.2 ([5]). *For all $\delta > 0$, there is a $s(\delta)$ such that if $s > s(\delta)$, for most primes p, there is a $n \in \mathcal{S}_{g,s}(\mathcal{D})$ such that $p \mid n$ and $\log n < p^{\delta}$.*

This was known for $\delta > 1/2$ (see [25]).

7.3 Mordell Type Estimate on Multiplicative Subgroups

Theorem 7.3 ([6]). *Let $G \lhd \mathbb{F}_p^*$, $|G| > p^{\delta}$ and $d > 0$ a fixed integer. Then*

$$\max_{(a_1,\ldots,a_d,p)=1} \left| \sum_{x \in G} e_p\big(a_1 x + a_2 x^2 + \cdots + a_d x^d\big) \right| < |G| p^{-\delta'} \ ,$$

with $\delta' = \delta'(\delta, d) > 0$.

7.4 Further Applications

Further applications of the method involve a full understanding of the sum-product theorem in product spaces $\mathbb{F}_p^2$. One may then establish a Mordell-type exponential sum estimate in basically optimal form.

Theorem 7.4 ([6]). *Let p be prime. Given $r \in \mathbb{Z}_+$ and $\varepsilon > 0$, there is a $\delta = \delta(r, \varepsilon) > 0$ satisfying the following property: If*

$$f(x) = \sum_{i=1}^{r} a_i x^{k_i} \in \mathbb{Z}[x] \quad \text{and} \quad (a_i, p) = 1 \ ,$$

where the exponents $1 \leq k_i < p - 1$ satisfy

$$\begin{aligned} (k_i, p-1) &< p^{1-\varepsilon} \quad \text{for all} \quad 1 \leq i \leq r \ , \\ (k_i - k_j, p-1) &< p^{1-\varepsilon} \quad \text{for all} \quad 1 \leq i \neq j \leq r \ , \end{aligned}$$

then there is an exponential sum estimate

$$\left| \sum_{x=1}^{p-1} e_p\big(f(x)\big) \right| < p^{1-\delta} \ .$$

Theorem 7.4 may be reformulated for exponential sums associated to power residues. In this setting, the result remains valid for incomplete sums, generalizing Theorem 5.4 to several generators $\theta_1, \ldots, \theta_r$. Thus

Theorem 7.5 ([6]). *Let $\theta_1, \ldots, \theta_r \in \mathbb{F}_p^*$ satisfy for some $\varepsilon > 0$ the estimates*

$$\begin{aligned} O(\theta_i) &> p^{\varepsilon} \quad \text{for all} \quad i = 1, \ldots, r \ , \\ O(\theta_i \theta_j^{-1}) &> p^{\varepsilon} \quad \text{for all} \quad 1 \leq i \neq j \leq r \ . \end{aligned}$$

Then, letting $t_1 > p^{\varepsilon}$

$$\max_{a_i \in \mathbb{F}_p^*} \left| \sum_{s=1}^{t_1} e_p \left(\sum_{i=1}^{r} a_i \theta_i^s \right) \right| < t_1 p^{-\delta} \ ,$$

with $\delta = \delta_r(\varepsilon)$.

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Perspectives and Challenges to Harmonic Analysis and Geometry in High Dimensions: Geometric Diffusions as a Tool for Harmonic Analysis and Structure Definition of Data

R.R. Coifman*

Department of Mathematics, Yale University, New Haven, CT 06520, USA
coifman@math.yale.edu

1 Introduction

Our goal is to describe some of the mathematical challenges confronted, when dealing with massive data sets. We point out that the trend set in hard analysis by L Carleson, of integrating combinatorics with geometry and harmonic analysis, is a powerful guide in the context of analytic geometry of data.

The task confronted by the scientist or engineer is to organize and structure enormously complex high dimensional clouds of points. More importantly, the scientist is challenged by the need to approximate empirical functions depending on many parameters effectively . Here effective methods are the ones for which the *complexity of the method does not grow exponentially with the dimension. In effect no tools from classical approximation theory and analysis exist.*

Various methods for embedding high dimensional data sets in relatively modest dimensions were introduced by various groups of researchers. In particular Johnson and Lindenstrauss have shown that N points in N dimensions can almost always be projected to a space of dimension $C \log N$ with control on the ratio of distances. J Bourgain has proved that any finite metric space with N points can be embedded by a bi-Lipschitz map into $\log N$ dimensional Euclidean space with bi-Lipschitz constant $\log N$. Various randomized versions of this theorem have become useful tools for protein mapping and other data analysis tasks. These results indicate that in practice to address the problem of functional approximation it would be enough to restrict our attention to dimensions below 50.

* The results in this talk are joint work with S. Lafon, A. Lee, M. Maggioni, S. Zucker.

2 Diffusion Geometries and Data Organization

The situation is not so difficult when dealing with clouds of points in high dimensions which are distributed near lower dimensional manifolds or varifolds. In particular empirical manifold learning is an active area of research.

We now would like to use Harmonic analysis as a tool to process empirical data sets.

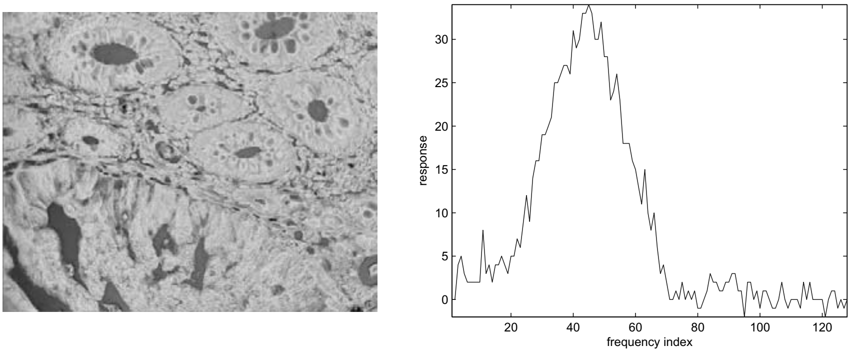

Fig. 1. Hyperspectral image of a pathology slide (left) with associated spectrum (right).

The hyperspectral image of a pathology slide to the left in Fig. 1 provides an illustration of some of the issues mentioned above, here to each pixel of the image is associated a spectrum (Fig. 1, right) representing the electromagnetic absorption of the tissue in 28 bands. This spectrum reflects the mix of biological constituents. The coloring in RGB of the image provides at each location a mix of three tissue types.

For physical reasons it is expected that these points in 28 dimensional space lie on different low dimensional submanifolds.

Our goal is to provide a general methodology to describe and parametrize it. Our method provides a framework for structural multiscale harmonic analysis on subsets (data) of $\mathbb{R}^n$ and on graphs. We use diffusion semigroups to generate multiscale geometries in order to organize and represent complex structures. We build the diffusions through an “infinitesimal” Markov process, and will show that the top eigenfunctions of the Markov operator permit a low dimensional geometric embedding of the data set into $\mathbb{R}^n$ so that the ordinary Euclidean distance in the embedding space measures intrinsic diffusion metrics on the data. Moreover we will indicate how empirical functions on the data can be naturally extended to all of space.

While some of these ideas appear in a variety of contexts of data analysis, such as spectral graph theory, manifold learning, nonlinear principal components and kernel methods. We augment these approaches by showing that the diffusion distances are key intrinsic geometric quantities linking spectral theory of the Markov process (Laplace operator, or Kernels) to the corresponding geometry of the data, relating localization in spectrum to localization in space, opening the door to the application of methods from signal processing to analyze functions and transformations on the data.

Initially, our goal is to describe efficiently (empirical) functions on a set Γ (data) or on a discrete graph. In particular we consider the analysis of restrictions of band limited functions to the data (i.e. functions whose Fourier transform is supported in a ball B). Specifically, the space of restrictions of band limited function to the data set Γ, is spanned by the eigenvectors of the covariance operator

$$k_B(x,y) = \int_B e_\xi(x)e_\xi(-y)\mathrm{d}\xi \ ,$$
$$\lambda_j\varphi_j = \int_\Gamma k_B(x,y)\varphi_j(y)\mathrm{d}y \ .$$

These eigenfunctions have natural extensions as band limited functions in $\mathbb{R}^n$ given by

$$\phi_j(x) = \frac{1}{\lambda_j}\int_\Gamma k_B(x,y)\varphi_j(y)\mathrm{d}y \ .$$

It turns out that $\phi_j(x)$ form an orthogonal set on $\mathbb{R}^n$ of band limited functions whose norm is maximized on the set (generalizing the classical prolate functions). For the example of the unit sphere these eigenfunctions are the spherical harmonics which are the eigenfunctions of the Laplace operator. We will refer to the extensions of these eigenfunctions as geometric harmonics (since these extensions are characterized as the minimal norm band limited extension of the given restriction to the set). We will use these extensions for estimating empirical regression off the data set.

More generally for data lying on a submanifold of $\mathbb{R}^n$, any restriction of a positive radial kernel leads to approximations of eigenfunctions of the Laplace–Beltrami operator on the manifold. We now extend results of Belkin et al. relating kernels and Laplace–Beltrami operators on submanifolds of Euclidean space.

We restrict a positive symmetric kernel to the data set, as an operator (or matrix)

$$K(f) = \int_\Gamma k(x,y)f(y)\mathrm{d}y$$

and diagonalize K as

$$k(x,y) = \sum \lambda_i^2\varphi_i(x)\varphi_i(y) \ .$$

Then

$$D^2(x,y) = k(x,x) + k(y,y) - 2k(x,y) = \sum \lambda_i^2\big(\varphi_i(x) - \varphi_i(y)\big)^2$$

is the square of the metric $D(x, y)$.

If the kernel is given as a function of some initially given metric $d(x, y)$ (for example d could be the geodesic metric), and $k(x, y) = k(d^2(x, y))$, $k'(0) = 1$, then

$$D(x, y) \approx \frac{d(x, y)}{1 + d(x, y)} = d_0(x, y) \; .$$

This observation shows that for data on a compact submanifold of $\mathbb{R}^n$, the kernel metric is equivalent to the original metric.

A particularly important case arises from a scaled weighted Gaussian kernel operator (by a density of point distribution $p(y)$)

$$\int_{\Gamma} \exp(-d(x, y)^2/\varepsilon) f(y) p(y) \mathrm{d}y \; .$$

This kernel has to be renormalized as follows; let

$$p_\varepsilon(x) = \int_{\Gamma} \exp(-d(x, y)^2/\varepsilon) p(y) \mathrm{d}y$$

and

$$\nu_\varepsilon(x) = \int_{\Gamma} \exp(-d(x, y)^2/\varepsilon) \frac{p(y) \mathrm{d}y}{p_\varepsilon(x)} \; .$$

Then the operator[2]

$$A_\varepsilon(f) = \int_{\Gamma} a_\varepsilon(x, y) f(y) p(y) \mathrm{d}y \; ,$$

where

$$a_\varepsilon(x, y) = \frac{\exp(-d(x, y)^2/\varepsilon)}{\nu_\varepsilon(x) p_\varepsilon(y)}$$

is an approximation to the Laplace–Beltrami diffusion kernel at time ε.

The operator A_ε can be used to define a discrete approximate Laplace operator

$$\Delta_\varepsilon = \frac{1}{\varepsilon}(A_\delta - I) = \Delta_0 + \sqrt{\varepsilon} R_\delta \; ,$$

where R is bounded on band limited functions and Δ_0 is the Laplace–Beltrami operator on the manifold. From this we can deduce the following theorem:

Theorem 2.1.

$$(A_\delta)^{t/\delta} = (I + \varepsilon \Delta_\delta)^{t/\delta} = (I + \varepsilon \Delta_0)^{t/\delta} + O(\sqrt{\varepsilon}) = \exp(t\Delta_0) + O(\sqrt{\varepsilon})$$

and the kernel of $(A_\delta)^{t/\delta}$ *is given as*

$$a_t(x, y) = \sum \lambda_i^{2t/\delta} \psi_i(x) \psi_i(y) = \sum \exp(-\mu_l t) \phi_l(x) \phi_l(y) + O(\sqrt{\varepsilon}) \; ,$$

where the ϕ *are the eigenfunctions of the limiting Laplace operator and all estimates are relative to any fixed space of band limited functions.*

[2] Shoenberg proved that this operator is positive, if and only if the metric d embeds isometrically in Hilbert space.

Strictly speaking we assume here that the data is relatively densely sampled (each ball of radius ε contains several points) on a closed compact manifold. In case the data only covers a sub domain of the manifold, the Laplace operator needs to be interpreted as the restriction of the Laplace operator with Neumann boundary condition.

The fundamental observation is that the numerical rank of the powers of A decreases rapidly (see Fig. 2 below) and therefore the diffusion distance given by

$$a_t(x,x) + a_t(y,y) - 2a_t(x,y) = D_t^2(x,y)$$

can be computed to high accuracy using only the corresponding eigenfunctions. This choice of an embedding into Euclidean space so as to convert diffusion distance on the manifold into Euclidean distance in the embedding will be called a diffusion map.

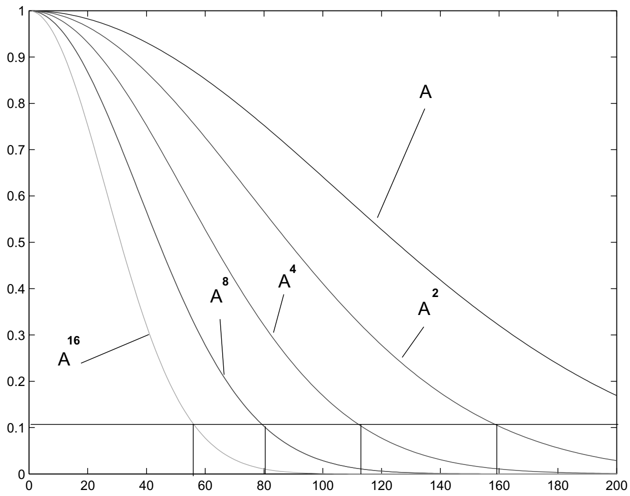

Fig. 2. Some examples of the spectra of powers of A.

We illustrate this point for the case of a closed rectifiable curve, for which the first two non constant eigenfunctions give a realization of the arc length parametrization onto the circle of the same length. In fact a simple computation relative to the arc length parametrization shows that the heat kernel is given by

$$e_t(x,y) = \sum \exp(-k^2 t) \cos\big(k(x-y)\big)$$

and

$$\mathrm{e}^t D_t^2(x,y) = |\mathrm{e}^{\mathrm{i}x} - \mathrm{e}^{\mathrm{i}y}|^2 \big(1 + \mathrm{e}^{-3t} r_t(x,y)\big) \ ,$$

where r is bounded.

In Fig. 3 we see points distributed (non uniformly) on the spiral on the left, the next embedding into the plane is given by the conventional graph Laplacian normalization, while the circle was obtained as above. The graph on the right is the density of points on the circle.

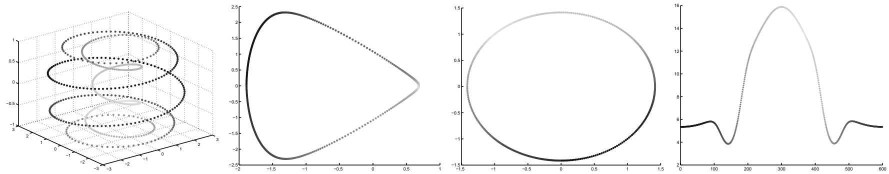

Fig. 3. From left to right: points distributed on a spiral—an embedding into the plane—a circle obtained as above—a graph depicting the density of points on the circle.

More generally we have the following theorem

Theorem 2.2. *Let $x_i \in \Gamma \subseteq M$ be a data set in the compact Riemannian manifold M so that each point in the manifold is at a distance ε from one of the data points and let the matrix $a_t(x,y)$ be defined as above on the data, with*

$$a_t(x,y) = \sum \lambda_i^{2t/\varepsilon} \psi_i(x)\psi_i(y) \, .$$

Then there exists an m such for all t sufficiently large the diffusion map is an embedding of M into m dimensional Euclidean space which is approximately isometric relative to the extrinsic Euclidean distance.

$$x \in M \mapsto \tilde{x} = \left(\lambda_1^{t/\varepsilon}\psi_1(x), \lambda_2^{t/\varepsilon}\psi_2(x), \dots \lambda_m^{t/\varepsilon}\psi_m(x)\right) \in \mathbb{R}^m$$

$$D_t^2(x,y) = \sum_{i=1}^{m} \lambda_i^{2t/\varepsilon}\left(\psi_i(x) - \psi_i(y)\right)^2\left(1 + O(\mathrm{e}^{-\alpha t})\right) = |\tilde{x} - \tilde{y}|^2\left(1 + O(\mathrm{e}^{-\alpha t})\right)$$

The proof of this theorem uses the fact that for small t and large m we have an embedding, we then pick the smallest m for which we have a bi-Lipschitz embedding and the next eigenvalue is strictly smaller (we can also maximize the spectral gap to have higher precision).

The next example (Fig. 4) embeds an hourglass surface into three dimensional Euclidean space so that the diffusion distance in embedding space between two points is the length of the chord connecting them.

Since the diffusion is slower through the bottle neck the two components are farther apart in diffusion metric.

Figure 5 illustrates the organizational ability of the diffusion maps on a collection of images that was given in random order as reordered by the mapping given by the first two nontrivial eigenfunctions.

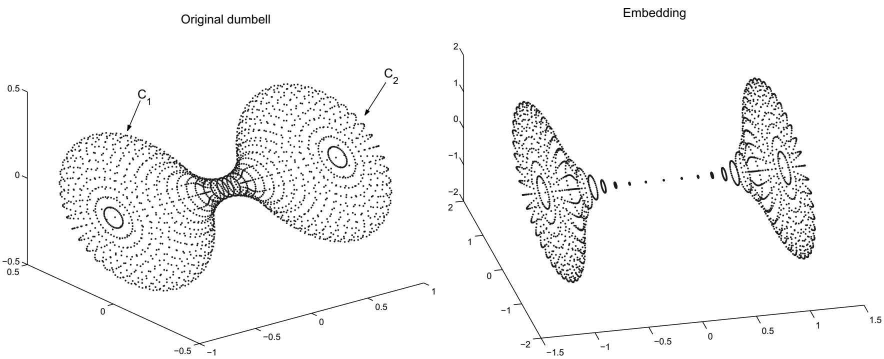

Fig. 4. Original dumbbell (left) and embedding (right).

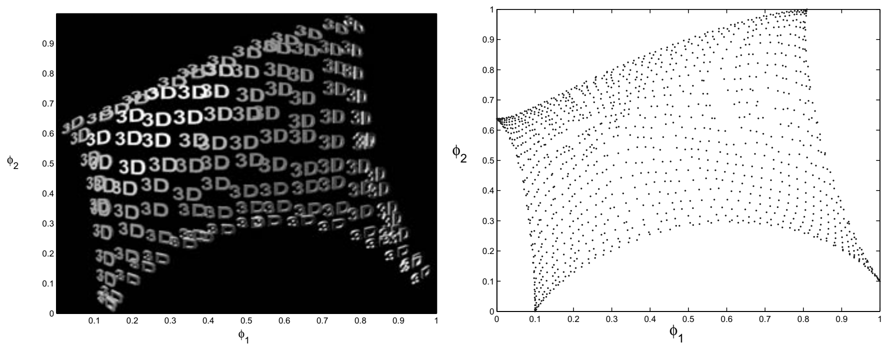

Fig. 5. The first two eigenfunctions organize the small images which were provided in random order.

Figure 6 shows the conventional nearest neighbor search compared with a diffusion search. The data is a pathology slide, each pixel is a digital document (spectrum below for each class).

3 Extension of Empirical Functions off the Data Set

An important point of this multiscale analysis involves the relation of the spectral theory on the set to the localization on and off the set of the corresponding eigenfunctions. In the case of a smooth compact submanifold of Euclidean space it can be shown that any band limited function of band B can be expanded to exponential accuracy in terms of eigenfunctions of the Laplace operator with eigenvalues μ^2 not exceeding CB.

Conversely every eigenfunction of the Laplace operator satisfying this condition extends as a band limited function with band $C'B$ (both of these state-

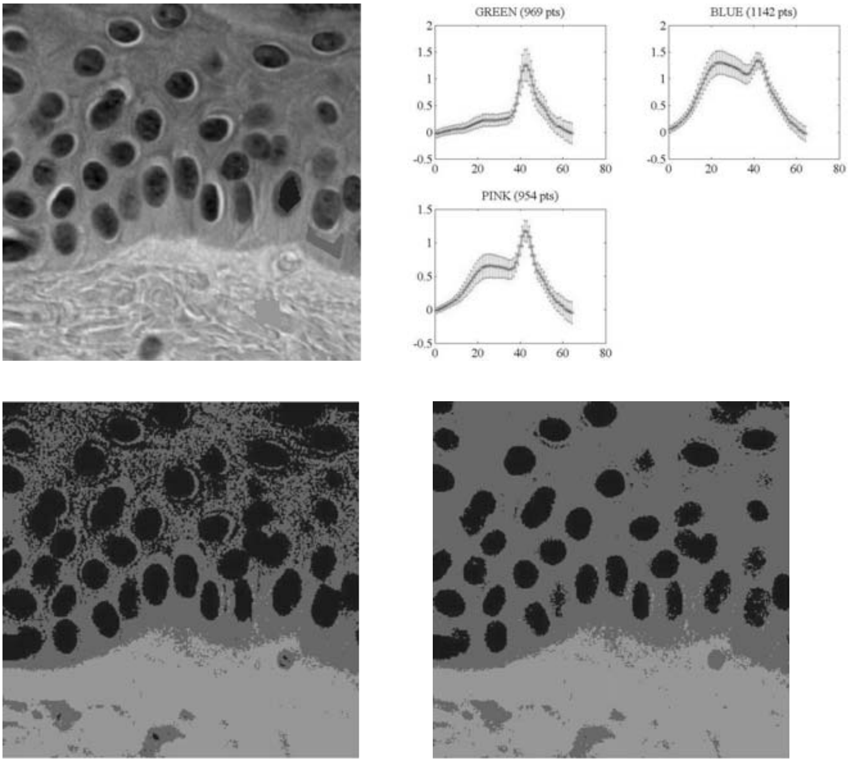

Fig. 6. Top-left to bottom-right: 256×256 image with 861 labeled points—spectrum for each class–nearest neighbor search—extension to all points.

ments can be proved by observing that we can estimate the size of a derivatives of order $2m$ of eigenfunctions of the Laplace operator as a power m of the eigenvalue). If we extend the eigenfunctions as constant in the normal direction to the submanifold (by introducing an appropriate smooth partition of unity in a neighborhood of the submanifold). It is easy to see that the Fourier transform at ξ of such an extension is estimated by $C_m(\mu/|\xi|)^m$ and this shows that eigenfunctions of the Laplace operator corresponding to eigenvalue μ on the manifold are well approximated by restrictions of band limited functions of band C_μ.

We conclude that given an empirical function on the manifold which can be approximated to some accuracy with eigenfunctions whose frequencies are localized, or which is expanded in terms of a multiscale basis involving eigenvalues of the Laplace operator not exceeding μ, then such a function can be extended as a band limited function off the set to a distance corresponding to $C\mu^{-1}$ and the best band limited approximation can be obtained from the corresponding Band limited projection kernel $k_B(x, y)$ defined above.

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Open Questions on the Mumford–Shah Functional

Guy David

Équipe d'Analyse Harmonique (CNRS), Université de Paris XI (Paris-Sud), 91405 Orsay, France guy.david@math.u-psud.fr

1 Introduction

The Mumford–Shah functional was introduced in [20] as a tool for image segmentation. In this context, we are given a simple domain Ω (the screen) and a bounded function g on Ω (representing the image), and we look for a simplified approximation u of g. Here simplified means that we would like u to have only slow variations on Ω, except that we want to allow jumps on a nice singular set K, which we think of as a set of boundaries. In the good cases, it is hoped that the pair (u, K), or even K or u alone, will retain important information on g and drop less interesting details or noise.

Mumford and Shah proposed to get image segmentations by minimizing the following functional, which we already define on $\mathbb{R}^n$ to save time (but so far image processing corresponds to $n = 2$). Set

$$J(u, K) = H^{n-1}(K) + \int_{\Omega\setminus K} |\nabla u|^2 + \int_{\Omega\setminus K} |u - g|^2 \ , \tag{1}$$

where we restrict to pairs (u, K) such that K is a closed set in Ω, with finite Hausdorff measure $H^{n-1}(K)$ of codimension 1, and u lies in the Sobolev space $W^{1,2}(\Omega \setminus K)$, which means that it has a derivative in L^2 on that open set. For the purpose of this lecture, it would be enough to restrict to $u \in C^1(\Omega \setminus K)$, because this is the case for minimizers, but this would be less natural.

The three terms in the functional correspond to the three constraints on u that were mentioned above, except perhaps that $H^{n-1}(K)$ does not really measure how simple K is. We shall return to this soon. In principle one should multiply two of the three terms by tuning constants, but we can normalize out one of them by multiplying u and g by a constant, and the other one by dilating everything.

The existence of pairs (u, K) for which $J(u, K)$ is minimal (we shall call them *minimizers*) is far from trivial, because we can easily find minimizing sequences $\{(u_k, K_k)\}$ that converge to pairs (u, K), but for which

$H^{n-1}(K) > \limsup_{k\to+\infty} H^{n-1}(K_k)$. Nevertheless, minimizers always exist; this was proved by Ambrosio [2] and De Giorgi, Carriero, Leaci [15].

Then we can ask what minimizing pairs look like. Let us first observe that when K is fixed, minimizing $J(u,K)$ in terms of u is rather simple. The two last terms of the functional are convex in u, so there is a unique minimizer; in addition this minimizer is rather regular (away from K), for instance because it satisfies the elliptic equation $\Delta u = u - g$ on $\Omega \setminus K$. As for regularity near K, the best way to get is to show first that K is nice. In this respect, it may help the reader to think about the special case of dimension 2 and the simpler local minimization of $\int_{\Omega\setminus K} |\nabla u|^2$ in $\Omega \setminus K$. In this case, we can use the fact that energy integrals are conformally invariant to map K locally into something nicer (like a line) by a conformal mapping ψ; the regularity of u will then depend mostly on the size of ψ'. The general case (with the extra term $\int |u-g|^2$ and in higher dimensions) is not very different.

So the main problem is the regularity of the singular set K. Observe that if we add a set of H^{n-1}–measure 0 to K, we do not change $J(u,K)$ but our description of K may become more complicated. For this reason we shall restrict to *reduced minimizers*, i.e., minimizers (u,K) for which we cannot find $K_1 \subset K$, $K_1 \neq K$, such that u has an extension in $W^{1,2}(\Omega \setminus K_1)$. It is rather easy to see that for each minimizer (u,K) there is a reduced minimizer (u_1,K_1) such that $K_1 \subset K$ and u_1 is an extension of u.

In dimension $n = 2$, Mumford and Shah conjectured that if (u,K) is a reduced minimizer for J and Ω is bounded and smooth, K is a finite union of C^1 arcs of curves, that may only meet by sets of three, at their ends, and with angles of $120°$. The reader should not pay too much importance to the precise statement, with the C^1 curves. The point is to get some minimal amount of regularity; once we know that K is a C^1 curve near a point, it is easy to get additional regularity (like $C^{1,1}$, see [5], and even better if g is smooth).

In higher dimensions, it is reasonable to expect that there is a set of codimension 2 in K out of which K is locally a C^1 hypersurface, but there is no very precise conjecture on the shape of that set of codimension 2. We shall return to this in Sect. 6.

Many partial results are known. We shall try to describe a few in the next sections, but the main goal of this text is rather to convince the reader that there are many interesting open questions besides the celebrated Mumford–Shah conjecture above; in addition, some of them could even be easy.

Before we move to a rapid discussion of known regularity results, let us observe that they are also good news for image segmentation. First they mean that even though we only put the term $H^{n-1}(K)$ in the functional, singular sets of minimizers are actually smoother than this term suggest, and in particular they look like what we would normally think boundaries in an image should look like. If minimizers for J had often been unrectifiable Cantor sets, J would probably have been much less used for image segmentation. Also, good regularity properties for minimizers probably mean better resistance to noise (because the functional cannot render noise, even if it tries to), and should help with the computations of minimizers, both because it should make them more stable and because we already know what to look for.

Nonetheless, it seems fair to say that J and its variants are a little less used in image segmentation nowadays, probably because people prefer to use algorithms that include some a priori knowledge, often of a statistical nature, on the images to be treated. See [18] and the references therein for more information on image processing.

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2 First Regularity Results

Let (u, K) be a reduced minimizer for J in a domain $\Omega \subset \mathbb{R}^n$. A first remarkable property of K is its local Ahlfors–regularity: there is a constant C, that depends only on n and $||g||_\infty$, such that

$$C^{-1} r^{n-1} \leq H^{n-1}(K \cap B(x,r)) \leq C r^{n-1} \tag{2}$$

when $x \in K$, $0 < r \leq 1$, and $B(x,r) \subset \Omega$. The second inequality is very easy (and does not require $B(x,r)$ to be contained in Ω): simply consider the competitor (v, G) obtained by keeping $G = K$ and $v = u$ out of $\overline{B}(x,r)$, setting $K = \emptyset$ and $v = 0$ in $B(x,r)$, and adding $\partial B(x,r) \cap \Omega$ to G to allow jumps across $\partial B(x,r)$. Thus we take $G = [K \setminus \overline{B}(x,r)] \cup [\partial B(x,r) \cap \Omega]$. When we write that $J(u,K) \leq J(v,G)$, we get that

$$\begin{aligned} H^{n-1}(K \cap B(x,r)) &+ \int_{\Omega \cap B(x,r) \setminus K} |\nabla u|^2 \\ &\leq H^{n-1}(\partial B(x,r) \cap \Omega) + \int_{B(x,r) \cap \Omega} |g|^2 \leq C r^{n-1} + C r^n ||g||_\infty^2 \, , \end{aligned} \tag{3}$$

which yields the second inequality in (2) when $r \leq 1$.

The first inequality in (2) is due to Dal Maso, Morel, and Solimini [8] when $n = 2$, and to Carriero and Leaci [7] in higher dimensions, and it is more subtle. It means that it does not help to put just a small amount of K somewhere, because it will not be enough to create big jumps across K and release the tension. That is, suppose we have a ball B such that $H^{n-1}(K \cap B)$ is very small; we want to say that you could do better by removing $K \cap B$ from the singular set. This will allow you to save $H^{n-1}(K \cap B)$ in the first term of J, but of course you will have to replace u in B with a function $\widetilde{u}$ that does not jump across $K \cap B$. A good choice is to take the harmonic extension of the values of u on ∂B. Then we can estimate how much larger $\int |\nabla \widetilde{u}|^2$ has to be (one shows that the contributions that come from the $|u-g|$ term can be neglected). An integration by parts shows that the price we have to pay is essentially the integral on $K \cap B$ of a product $\mathrm{Jump}(u) \times \frac{\partial \widetilde{u}}{\partial n}$, of the jump of u across $K \cap B$ times the derivative of $\widetilde{u}$ in a direction perpendicular to K. The computations can essentially be done like this when $n = 2$, and this is the essence of the proof in [8]. The point is that the jump of u can be estimated, and it is at most $CH^1(K \cap B)^{1/2}$. Then the integral of $\mathrm{Jump}(u) \times \frac{\partial \widetilde{u}}{\partial n}$ is much smaller than $H^1(K \cap B)$, and we get the desired contradiction. When $n > 2$, complications appear, in particular because we may not be able choose B so that $\partial B \cap K$ is empty, and the proof of [7] uses a compactness argument.

Notice that (2) is already good to know for image processing.

We talked a lot about (2) because it is a very useful tool for proving other estimates, for instance because it says that K is a space of homogeneous type. Let us just give an example. Set

$$\omega_p(x,r) = r^{1-2n/p} \left\{ \int_{B(x,r) \setminus K} |\nabla u|^p \right\}^{2/p} , \tag{4}$$

for $1 \leq p \leq 2$, $x \in K$, and $B(x,r) \subset \Omega$; do not pay too much attention to the normalizations, the main point is to have a dimensionless quantity. The trivial estimate (3) says that $\omega_2(x,r) \leq C$ for $r \leq 1$, but with (2), (3), Hölder, and Fubini, one can readily show the Carleson measure estimate

$$\int_{y \in K \cap B(x,r)} \int_{t=0}^{r} \omega_p(y,t) \, \frac{dH^{n-1}(y)\mathrm{d}t}{t} \leq C_p r^{n-1} , \tag{5}$$

for $x \in K$ and $0 < r \leq 1$ such that $B(x,3r) \subset \Omega$, provided that we take $p < 2$ [12]. It often turns out that replacing 2 with a smaller exponent p is a very small price to pay, compared to the fact that (5) gives lots of pairs such that $\omega_p(y,t)$ is as small as we want. For instance (5) is a very good starting point for the results quoted just below; the good balls mentioned below are precisely balls where $\omega_p(y,Ct)$ is small.

Next (and omitting quite a few interesting results), K is locally uniformly rectifiable and contains big pieces of Lipschitz graphs ([12], [14]). But even more is true ([9], [3], [21]): we can find lots of balls where K is C^1. More precisely, there is a constant C such that, for each $x \in K$ and $r \in (0,1]$ such that $B(x,r) \subset \Omega$, we can find $y \in K \cap B(x,r/2)$ and $t \in [r/C, r/2]$ such that $K \cap B(y,t)$ is the intersection of $B(y,t)$ with the graph of a 10^{-2}–Lipschitz and C^1 function.

As a consequence there is a small set, in fact of Hausdorff dimension less than $n-1$, out of which K is locally nice and C^1. But we would like to know more about that small set, and the way the different pieces are attached to each other.

See [4], [10], [13], [18] and their references for proofs and lots of other regularity results on K. Here we shall just say a little more about a result of Bonnet [5]:

Fact 2.1. In dimension 2, every *isolated* connected component of K is a finite union of C^1 curves.

The reason why we mention this is because the approach that led to it is very important. Notice that Fact 2.1 is much more precise than the C^1 result mentioned above, but only if we can find an isolated component.

3 Blow-up Limits and Global Minimizers

We start with a very simple observation on dilation invariance. Pick a point $x \in \Omega$ (typically, $x \in K$) and a small radius t, and dilate everything so that $B(x,t)$ becomes the unit ball. That is, set $\Omega_{x,t} = t^{-1}(\Omega - x)$, $K_{x,t} = t^{-1}(K - x)$, $g_{x,t}(y) = \frac{1}{\sqrt{t}}\, g(x+ty)$ for $y \in \Omega_{x,t}$, and $u_{x,t}(y) = \frac{1}{\sqrt{t}}\, u(x+ty)$ for $y \in \Omega_{x,t} \setminus K_{x,t}$. We divided by $\sqrt{t}$ so that the two first terms of J in (1) would scale the same way. A simple computation shows that if (u,K) minimizes J, $(u_{x,t}, K_{x,t})$ is a minimizer for $J_{x,t}$, where

$$J_{x,t}(v,G) = H^{n-1}(G) + \int_{\Omega_{x,t}\setminus G} |\nabla v|^2 + t^2 \int_{\Omega_{x,t}\setminus G} |v - g_{x,t}|^2 \,. \tag{6}$$

Notice that when t gets small, the third term becomes less and less important, even though $||g||_\infty^2$ is divided by t. This corresponds to the (desired for image segmentation) effect that the third term of J in (1) should have little influence at small scales, and is one of the basic facts of the theory. It is thus surprising that we had to wait till [5] before one actually decided to take blow-up sequences and study their limits, as follows.

Fix a point $x \in K$, and take a sequence $\{t_k\}$ that tends to 0. Set $(u_k, K_k) = (u_{x,t_k}, K_{x,t_k})$ to simplify notation. One hopes that limits of such pairs are simpler, and that they will help us study (u,K).

The first thing to check is that given any sequence $\{(u_k, K_k)\}$ as above, we can extract subsequences that converge. Note that Ω_{x,t_k} converges to $\mathbb{R}^n$, so the limits should be pairs (v,G) that live on $\mathbb{R}^n$.

We do not have too much choice when defining the convergence of $\{K_k\}$ to a limit K_∞; if we want to be sure to have convergent subsequences, we have to use the local convergence in Hausdorff distance, which is also the most reasonable notion. The convergence of $\{u_k\}$ to v is a little more delicate to define, because the L^∞ norms of the u_k will normally tend to $+\infty$. On the other hand, we have a good uniform control on the gradients away from G, by (3), so we just require the convergence of the gradients ∇u_k in some L^p, on compact subsets of $\mathbb{R}^n \setminus G$. Equivalently (and this is the definition used in [10]) we require the following property.

Property 3.1. For each connected component V of $\mathbb{R}^n \setminus G$, there exists constants $\alpha_{V,k}$ such that $\{u_k - \alpha_{V,k}\}$ converges to v in $L^1(H)$ for every compact subset H of V.

This looks a little strange at first, because we have to subtract constants (and then v in only known up to an additive constant in each component of $\mathbb{R}^n \setminus G$), but this is the right way to deal with the fact that $||u_k||_\infty$ tends to $+\infty$.

With these definitions, it is not hard to extract convergent subsequences from any $\{(u_k, K_k)\}$ as above. One of the main points of [5] is the following.

Fact 3.2. If (u, K) is a reduced minimizer for J and $\{(u_k, K_k)\}$ converges to (v, G), then (v, G) is a reduced global minimizer in $\mathbb{R}^n$.

We shall see the definition in a moment, but let us first comment a little. First of all, Fact 3.2 is not trivial, once again because its verification involves checking that

$$H^{n-1}(G \cap U) \leq \lim_{k \to +\infty} H^{n-1}(K_k \cap U) \ , \tag{7}$$

for every open set $U \subset \Omega$, and this would brutally fail for a general sequence of sets K_k. But it turns out that since the K_k come from Mumford–Shah minimizers, they have a very nice property, the so-called uniform concentration property.

To simplify things slightly, we shall say that this property holds when, for every $\varepsilon > 0$, we can find $C > 0$ such that, for each ball $B(x, r)$ contained in Ω, centered on a K_k, and with radius $r \leq 1$, we can find another ball $B(y, t) \subset B(x, t)$, centered on the same K_k, with radius $t \geq C^{-1} r$, and for which we have the nearly optimal concentration

$$H^{n-1}(K_k \cap B(y, t)) \geq (1 - \varepsilon)\, \omega_{n-1}\, t^{n-1} \ , \tag{8}$$

where ω_{n-1} is the H^{n-1}–measure of the unit ball in $\mathbb{R}^{n-1}$. Thus the measure in (8) is at least almost as large as if K_k were a hyperplane through y. Then (7) holds as soon as the uniform concentration property holds.

We simplified things a little, because the uniform concentration property of [8] also allows us to modify slightly the quantifiers above (but the important thing is still to keep C independent of k); also their result still works in (integer) dimensions $d < n - 1$. See [8] or [18] for details.

Uniform concentration was introduced in [8], and proved for minimizers in [8] when $n = 2$ and [22] when $n > 2$. Also see in [10] for a proof with uniform rectifiability.

Once we get the semicontinuity of Hausdorff measure as in (7), the rest of the proof of Fact 3.2 is a technical, but not surprising argument. See [5] for the initial proof in two dimensions, [16] for a first generalization, and [17], [10] for extensions to higher dimensions and different limiting situations.

It is time to define global minimizers. Let us only consider "acceptable pairs" (v, G) such that G is a closed subset of $\mathbb{R}^n$, $v \in W^{1,2}_{loc}(\mathbb{R}^n \setminus G)$, and in addition

$$H^{n-1}(G \cap B(0,R)) + \int_{B(0,R)\setminus G} |\nabla v|^2 < +\infty \, ,$$

for every $R > 0$. A competitor for (v, G) is another acceptable pair $(\widetilde{v}, \widetilde{G})$ such that for R large enough, the pair $(\widetilde{v}, \widetilde{G})$ coincides with (v, G) out of $\overline{B}(0, R)$, and in addition G satisfies the following topological condition.

Property 3.3. If $x, y \in \mathbb{R}^n \setminus [G \cup \overline{B}(0,R)]$ lie in different connected components of $\mathbb{R}^n \setminus G$, then they lie in different connected components of $\mathbb{R}^n \setminus \widetilde{G}$.

We say that the acceptable pair (v, G) is a *global minimizer* if

$$H^{n-1}(G \cap \overline{B}(0,R)) + \int_{B(0,R)\setminus G} |\nabla v|^2 \\ \leq H^{n-1}(\widetilde{G} \cap \overline{B}(0,R)) + \int_{B(0,R)\setminus \widetilde{G}} |\nabla \widetilde{v}|^2 \, , \quad (9)$$

for every competitor $(\widetilde{v}, \widetilde{G})$ for (v, G), and R as above. Note that (9) does not depend on R large.

The topological constraint of Property 3.3 on competitors may seem a little strange, but it is imposed to us by the fact that we needed to work modulo constants when taking limits. If we did not ask for Property 3.3, taking for G a straight line and v a locally constant function on $\mathbb{R}^2 \setminus G$ would not give a global minimizer. This would be bad, because we know that such a pair shows up each time you take the blow-up limit of a Mumford–Shah minimizer (u, K) at a point where K is a C^1 curve.

So we have a definition of global minimizers, and we define reduced global minimizers as we did for Mumford–Shah minimizers in a domain. Thus Fact 3.2 makes sense.

Our big hope, once we have Fact 3.2, is that global minimizers in $\mathbb{R}^2$, for instance, will turn out to be so simple that we can list them completely (and later return to the Mumford–Shah minimizers in a domain if we are still interested). Of course the definition of global minimizer is a little more complicated, because of this strange Dirichlet condition at infinity where (v, G) itself gives the Dirichlet data, but at least we lost the auxiliary function g and we have just two terms to worry about.

4 Global Minimizers in the Plane

Here is a list of global minimizers in the plane. For the first three, we take $v = 0$, or equivalently v constant on each component of $\mathbb{R}^2 \setminus G$. This works if and only if G is a minimal set. Here our definition of minimal set, suggested by Property (3.3) and (9), is that you cannot make it shorter by compact modifications that do not merge the connected components near infinity. But it is easy to see that it is equivalent to the more usual notion, where we say that we cannot make G shorter by deforming it in a bounded region. The only options for G are the empty set, or a line, or the union of three half lines with a same origin, and that make angles of $120°$ with each other (we shall call this a Y). In these three cases the verification that (v, G) is a reduced global minimizer is rather easy.

There is a fourth known type of global minimizer, where G is a half line. By translation and rotation invariance, we may assume that G is the negative first axis $\{(x, 0)\,;\, x \leq 0\}$; then we take

$$v(r\cos\theta, r\sin\theta) = \pm\sqrt{\frac{2r}{\pi}}\,\sin(\theta/2) + C\ , \tag{10}$$

for $r > 0$ and $-\pi < \theta < \pi$, where the choice of constants $\pm$ and C does not matter.

It is not too hard to see that (when G is the half line) the only choices of v for which (v, G) is a global minimizer must given by (10), but the verification that (10) gives a global minimizer is long and painful [6].

Here is the natural analogue of the Mumford–Shah conjecture in the present context.

Conjecture 4.1. Every reduced global minimizer in the plane is of one of the four types described just above.

Conjecture 4.1 implies the Mumford–Shah conjecture. See [10], but this was essentially known by Bonnet [5], who only wrote down the part he needed to show that the result quoted below (when G is connected) implies Fact 2.1.

A priori Conjecture 4.1 is a little stronger, because there could be global minimizers in the plane that do not arise as blow-up limits of Mumford–Shah minimizers in a domain. But it is hard to imagine that the Mumford–Shah conjecture will be proved without Conjecture 4.1.

Only partial results are known so far. Here is a short list; see [10] and [17] for more.

If (v, G) is a reduced global minimizer in $\mathbb{R}^n$, then G is Ahlfors–regular, uniformly rectifiable, and we can even find lots of balls centered on G where G is a 10^{-2}–Lipschitz and C^1 graph. The statements and proofs are the same as in the local case in the domain, except that we no longer need the restrictions that $r \leq 1$ or $B(x, r) \subset \Omega$.

Conjecture 4.1 holds when

- G is connected [5],
- G is contained in a countable union of lines [16],
- G is symmetric with respect to the origin [11], [17],
- $\mathbb{R}^2 \setminus G$ has at least two connected components, or when G contains two disjoint connected unbounded sets [11].

Many of the results listed here use a monotonicity argument, in addition to the usual techniques of finding alternative competitors. Again the trend started in [5], where one of the main ingredients of the proof was to show the following.

Fact 4.2. If (v, G) is a global minimizer in $\mathbb{R}^2$ and G is connected, then

$$\Phi(r) = \frac{1}{r}\int_{B(x,r)\setminus G} |\nabla v|^2$$

is a nondecreasing function of r, for each $x \in \mathbb{R}^2$.

This was proved by computing Φ', integrating by parts, and then using an inequality of Wirtinger. But (unfortunately) the connectedness of K was used to remove the mean value of u in some intervals, and it seems to be really needed in the argument.

Things become easier once you have Fact 4.2, because the proof of Fact 4.2 also gives the form of (u, K) when Φ is constant. This can be used to control blow-up and blow-in limits of (v, G), because the analogue of Φ for those is constant. Then we get a better local description of (u, K), and we can use it to conclude. The proof takes some time though. The improvement of the situation when we have a monotonicity result like Fact 4.2 should probably be compared with what happens with minimal surfaces, where an analogous monotonicity result implies that the tangent objects to the set are minimal cones.

In [11] also one shows monotonicity, but for the different function $\Psi(r) = 2\Phi(r) + r^{-1}H^1(G \cap B(x,r))$. The proof uses a combination of the Bonnet estimate and direct comparison with various competitors constructed by hand.

J.-L. Léger [16] found a nice formula that allows you to compute v in terms of G (modulo the obvious invariance of the problem) when (v, G) is a global minimizer in $\mathbb{R}^2$. Identify $\mathbb{R}^2$ with the complex plane, and set

$$F(z) = \frac{\partial v}{\partial x} - \mathrm{i}\frac{\partial v}{\partial y} = 2\frac{\partial v}{\partial z} \, ,$$

for $z \in \mathbb{R}^2 \setminus G$. Notice that F is holomorphic in $\mathbb{R}^2 \setminus G$, because v is real and harmonic. Léger says that F^2 is the Beurling transform of $H^1_{|G}$, i.e.,

$$F(z)^2 = -\frac{1}{2\pi}\int_G \frac{dH^1(w)}{(z-w)^2} \quad \text{for } z \in \mathbb{R}^2 \setminus G \, . \tag{11}$$

Finally, let us mention that global minimizers in a half plane $\mathbb{P}$ are easier to characterize: the only possibilities for G are the empty set, or a half line starting from $\partial\mathbb{P}$ and perpendicular to it, and in both cases v is constant on each component of $\mathbb{P} \setminus G$. We can use this to return to Mumford–Shah minimizers in a bounded smooth domain and prove that near $\partial\Omega$, K is only composed of C^1 curves that meet $\partial\Omega$ perpendicularly. See [17] or [11] and [10].

See [10] and its references for more results about global minimizers.

5 General Questions

We start with a few questions in the plane. Besides the Mumford–Shah conjecture (or partial questions), of course.

There is no uniqueness in general for minimizers of the Mumford–Shah functional. For instance, if you take $\Omega = \mathbb{R}^2$ and g equal to the characteristic function of $B(0,r)$, there is one value of r for which J has exactly two minimizers, one with $K = \partial B(0,r)$ and one with $K = \emptyset$. See for instance [13] or [10]. It is easy to construct lots of examples of the same type, where the lack of uniqueness comes from a jump in the solution. But maybe we still have uniqueness for generic data g. This question also holds in $\mathbb{R}^n$.

We do not know yet that the global minimizer in (10) ever shows up as the blow-up limit of some Mumford–Shah minimizer in a domain. Even if we restrict to $\Omega = B(0,1)$ and take $g = v$, we do not know how to show that the restriction of (v,G) to Ω minimizes J. See [1] for the corresponding positive answer for a Y.

Suppose that the minimizer in (10) is a blow-up limit at x of the Mumford–Shah minimizer (u,K) in a domain Ω. We know that in a pointed neighborhood of x, K is a C^1 curve that looks flatter as we get near x (see for instance Sect. 69 of [10]), but we do not know precisely how K behaves at x (is the curve C^1 up to x, or can it turn infinitely many times around x, for instance?).

The easier case of a half plane suggests that it may be interesting to look at global minimizers in other planar domains, or even in larger 2–dimensional surfaces. So far we only know about sectors with aperture $< 3\pi/2$ [11].

Many of the partial results in the plane become questions in higher dimensions. For instance, it is not known whether every connected component of $\mathbb{R}^n \setminus G$ is a John domain with center at infinity; we just know that they are unbounded. Or whether v can be constant in a component of $\mathbb{R}^n \setminus G$ without being constant on every component. When $n = 2$, these things are true, and we even know that $\mathbb{R}^2 \setminus G$ is connected in the interesting cases.

We would also like to generalize some of our perturbations results. We know from [3] that if (u,K) is a Mumford–Shah minimizer or a global minimizer, in any dimension, and if $B(x,r)$ is a small ball centered on K where K is very flat (i.e., close to a plane) and $r^{1-n} \int_{B(x,r)} |\nabla u|^2$ is very small, then $K \cap B(x,r/2)$ is a nice C^1 hypersurface, i.e., a C^1 perturbation of a plane. We would like to know whether in such a statement, we can replace planes with other minimal sets. We know about the case of the Y in the plane [9], and we would like to know about the product of the Y with a line (in $\mathbb{R}^3$), for instance. This would also be an excuse for understanding these minimal sets better.

A little more difficult would be to obtain analogues of the result that says that if some blow-in limit of the global minimizer (v,G) is the cracktip minimizer from (10), then (v,G) itself is as in (10) [6]. All these things should be useful if we want study global minimizers systematically, or go from results on global minimizers to their counterpart for minimizers in a domain.

Can a same set G correspond to two really different global minimizers (i.e., that would not be obtained from each other by multiplying v by ± 1 and adding a constant to it in each component of $\mathbb{R}^n \setminus G$)? When $n = 2$, this is impossible because of the formula (11).

Could it be that when we take complex or vector-valued functions, we get fundamentally new global minimizers? We do not know this even in the plane, but it seems even more unlikely there.

6 What is the Mumford–Shah Conjecture in Dimension 3?

We would also like to have a description of all global minimizers in $\mathbb{R}^3$, even if we can't prove it. Let us already enumerate the ones we know.

We start with the case when g is locally constant, and hence G is a minimal set. Jean Taylor essentially showed that there are only four possibilities: the empty set, a plane, the product of a Y with an orthogonal line (i.e., three half planes that meet along their common boundary with $120°$ angles), and a set composed of six faces bounded by four half lines that start from the same origin and make maximal equal angles with each other. [Think about dividing a regular tetrahedron into for equal parts that all touch the center and three vertices.] These are the same sets that show up as tangent objects to soap films.

We also get a global minimizer in $\mathbb{R}^3$ by taking the product of the cracktip in a plane (as in (10)) by an orthogonal line (so that v, for instance, will not depend on the last variable); the verification is rather easy.

Now it seems that there should be at least one other global minimizer, and it is not too obvious to guess what it should be.

Let us first try to say why we may think that the list above is not complete. The argument will be vague and indirect, but there are not many arguments in the other direction either.

Consider the Mumford–Shah functional J in the domain $\Omega = B(0,1) \times (-N, N) \subset \mathbb{R}^3$ and with a function g of the form $g(x,y,z) = \varphi(z)\, g_0(x,y)$, where φ is a smooth function such that $0 \leq \varphi \leq 1$, $\varphi(z) = 1$ for $z \leq -1$, and $\varphi(z) = 0$ for $z \geq 1$. To define g_0, let Y be the intersection with $B(0,1) \subset \mathbb{R}^2$ of the union of three half lines starting from the origin and making $120°$ angles. Call D_1, D_2, and D_3 the three connected components of $B(0,1) \setminus Y$, and set $g_0(x,y) = 2j - 2$ on D_j. We take N reasonably large, to make sure that the last term of J will have some importance in the discussion.

If we restricted to the smaller domain $B(0,1) \times (-N, -1)$, (u, K) would coincide with $(g, Y \times (-N, -1))$. This is because (g_0, P) is the only minimizer of the 2–dimensional analogue of J where $g = g_0$, by [1]; the argument for the reduction to the plane is the same as for the cracktip minimizer just above.

It is reasonable to think that $K \cap [B(0,1) \times (-N, -N/2)]$, say, looks a lot like $Y \times (-N, -N/2)$, with three almost vertical walls that meet along a curve γ with 120° angles. If there is no other global minimizers than the five mentioned above, all the blow-up limits of (u, K) are among the five. If in addition we have a perturbation theorem for the case when K is close to the product of a Y by a line, we should be able to follow the curve γ (where the blow-up limits of K are products of Y's by lines), as long as no other type of blow-up limit shows up on γ. We cannot really exclude the possibility that this never happens, because γ may go all the way to $\partial\Omega$. However, it seems very unlikely that γ will go all the way to the top boundary (because $g = 0$ on the top part of Ω; there would be no good reason for the existence of three high walls), and still unlikely that γ will turn and hit the side of $\partial\Omega$ (even though our function g is not symmetric).

So let us assume that γ ends somewhere in Ω, at a point x_0 where some other blow-up limit shows up. If we get the minimal set with six faces, and we have a perturbation theorem near this minimal set, there will be three new curves like γ that leave from x_0, and we can try to follow them again. The case when all curves eventually end up on $\partial\Omega$ also seems unlikely: it is not clear why it would be needed to isolate three components near the bottom, rather than allowing gentle variations of u. But this is definitely a weak point of the argument. Anyway, if this does not happen, some other blow-up limit shows up, with a global minimizer that is not in the list above. Obviously some numerical experiments could be useful here.

Let us even try to guess what the set G for this new global minimizer should look like. The simplest bet would be to take something like $Y \times (-\infty, 0]$, but this may be a little too naive. For one thing, even though $Y \times (-\infty, 0]$ is nicely invariant under rotations of 120°, the corresponding function v could not be (the increments of v along an orbit of 3 points always add up to 0, so they cannot all be equal or opposite). So, if there is a global minimizer (v, G) with $G = Y \times (-\infty, 0]$, we are sure to lose the essential uniqueness of v given G. This is not so bad in itself, but since the function g will not be rotation invariant anyway, it does not seem so important to require G to be invariant. Probably making one of the walls a little higher than the others could help accommodate the corresponding slightly larger variations of v along that wall.

The author's bet is that there is indeed one more global minimizer, where G is the cone over three arcs of great circle $\Gamma_i \subset \mathbb{S}^2$; the Γ_i are vertical, start from the south pole where they make angles of 120°, and there are two shorter ones and a longer one. The lengths should be determined by all sorts of constraints, the main one being that we also guess that v will be homogeneous of degree $1/2$, and we know it must be harmonic with Neumann boundary conditions $\frac{\partial v}{\partial n} = 0$. All these suggestions are based on essentially nothing, so the reader may find it fun to make any other bet. For instance, that there is a global minimizer for which function $\lambda \to \mathrm{e}^{-\lambda/2} v(\mathrm{e}^{\lambda} x)$ is almost periodic (but not periodic), or has a period $\sqrt{2}$. [Added in proof: since the lecture, Benoit Merlet did computations that indicate that the most obvious scenario suggested by the author is impossible.]

Our difficulty with rotations of order 3 leads us to wonder whether the situation would be different with functions v valued in $\mathbb{R}^2$, because then v could be rotation invariant. This seems tempting because we like symmetry, but I don't think this is too serious.

The interested reader may consult Sects. 76 and 80 of [10] for a few additional questions, or details about the questions above.

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Multi-scale Modeling

Björn Engquist

KTH, Nada, SE-100 44 Stockholm, Sweden and Department of Mathematics, University of Texas at Austin, Austin, TX 78712-1082, USA
engquist@nada.kth.se and engquist@ices.utexas.edu

In honor of Lennart Carleson on his 75th birthday

Summary. If a mathematical model contains many different scales the computational cost for its numerical solution is very large. The smallest scale must be resolved over the distance of the largest scale. A huge number of unknowns are required and until recently many such problems could not be treated computationally. We will discuss a new set of numerical techniques that couples models for different scales in the same simulation in order to handle many realistic multi-scale problems. In most of this presentation we shall survey existing methods but we shall also give some new observations.

1 Introduction

Multi-scale problems naturally pose severe challenges for scientific computing. The smaller scales must be well described over the range of the larger scales. Multi-scale objects must thus typically be resolved by a very large set of unknowns. The larger the ranges of scales, the more unknowns are needed and the larger the computational cost. Even with the power of todays computers many such problems cannot be treated by traditional numerical methods.

The notion of scales in the physical world is quite intuitive. As an example, the flow of the air in a room on the scale of meters and seconds depends on the details of smaller swirling eddies. The motion of these eddies depends on the interaction of molecules on substantially finer scales in space and time. We can go further and see how the forces between the molecules depend on the motion of electrons on scales of 10^{-15} seconds in time and less than 10^{-10} meters in space.

The distribution of scales in a function can naturally be defined mathematically by its Fourier transform or by other scale-based representations. One recent such example is wavelet decomposition. In some of our examples below we will use scaling laws to define functions with different scales. The function $f_\varepsilon(x)$ is said to have scales of orders 1 and ε when,

$$f_\varepsilon(x) = f(x, x/\varepsilon) , \qquad f(x,y)\text{: 1–periodic in } y . \tag{1}$$

If the ε–scale is localized, as in the physical example of a boundary layer, a mathematical model can be the following,

$$f_\varepsilon(x) = f(x, x/\varepsilon) , \qquad f(x,y) \to F(x), \text{ as } y \to \infty,\ y \geq 0 . \tag{2}$$

Typically, a narrow range of scales is modeled by effective equations for that particular range. Turbulence models would then describe the coarsest scales of the flow phenomena mentioned above. The finer scales could be approximated by the Navies–Stokes equations, the Boltzmann equation and the Schroedinger equation respectively. For many processes such effective equations does not exist and it is those that we are focusing on in this presentation. For convenience we restrict most of our discussion to problems with mainly two scales as in (1) and (2) above and let the $O(1)$ scale be the macro-scale and $O(\varepsilon)$ the micro-scale. This setting is quite common with the macro-scale the continuum scale and the micro-scale the atomistic scale. There are also many such examples in biology.

Ideally, we are able to derive an effective equation for the scale we are interested in. This equation should include the influence from all other scales in the original multi-scale problem. A classical example is geometrical optics as an approximation to high frequency wave propagation. Very often this derivation is done in the applied sciences but there are also general mathematical techniques as, for example, homogenization of partial differential equations, [2] and averaging of dynamical systems, [1].

We will consider the challenging and common cases when such focused effective equations are not available. In Sect. 2 we will discuss the computational cost for multi-scale simulations. Mathematically this touches on numerical error estimation and information theory. After a few comments on the evolution of scientific computing as a background we shall discuss standard numerical multi-scale methods in Sect. 4. In this traditional class of methods the full multi-scale problem is discretized and highly efficient numerical methods are then applied to accurately compute the full range of scales.

In a more recent type of computational multi-scale methods only a fraction of the micro-scale space is included in order to restrict the number of unknowns. This is needed when the range of scales is very large as it is in many realistic applications. The macro-scale and the micro-scale are coupled during the calculation in such a way that the overall computational cost is minimal. The micro-scale is not described all over the full domain of the independent variables but only sampled in order to give the necessary input to the macro-scale model. A good example of this new class of methods is the quasi-continuum method by Tadmor and collaborators, [14]. This technique couples a continuum model to molecular dynamics. We shall present a framework for these methods in the final section.

As an example of the sampling technique we shall also give a new method for very fast Fourier transform. This method has simple stochastic features. For other stochastic multi-scale models see the work of E and collaborators [8]. Compare the comments by Carleson in [5] regarding stochastic analysis in the application of mathematics.

2 Computational Complexity

Let us start with discussing computational complexity since that is the reason for why special multi-scale methods are being developed. We mentioned in the introduction the computational challenge of mathematically describing multi-scale processes. Just in order to represent a band limited real function of one real variable over the length of order 1 and with the smallest wavelength ε we need $O(\varepsilon^{-1})$ data points, Shannon [13]. We first give a simple direct estimate that the process of a traditional numerical solution for a multi-scale function typically requires even more unknowns and more arithmetic operations. We will however see in Sect. 2.2 that there are opportunities for reduction in the complexity if the functions have some added structure as for example scale separation.

2.1 Complexity of Numerical Algorithms

With computational complexity we will here mean the number of arithmetical operations that are needed to solve for an unknown function to the accuracy δ, measured in an appropriate norm. A typical estimate for a quadrature method or discretizations of differential or integral equations is,

$$\#\mathrm{op} = O(N(\varepsilon)\varepsilon^{-1})^{dr} = O(\varepsilon^{-dr(s+1)}) \leq C\varepsilon^{-d}\,. \tag{3}$$

Here $N(\varepsilon) = O(\varepsilon^{-s})$ denotes the number of data points per wavelength of the unknown function that is needed for a given error tolerance. This depends on the numerical methods and, for example, on the regularity of the solution. The number of dimensions is d and thus the total number of unknowns are at least $O(\varepsilon^{-d(s+1)})$. The exponent r depends on the numerical method and determines the number of operations that is required for a given number of unknowns. For an explicit method where the solution is given by a finite number operations per unknown, $s = 1$. If a Gaussian elimination with a dense matrix is required: $s = 3$. The reduction of the exponent r to a value close to one is the goal of the classical numerical methods mentioned in Sect. 4.

There has to be at least 2 data points per wave length and thus $N(\varepsilon) \geq 2$, [13]. More unknowns are often required to achieve a given accuracy with, $N(\varepsilon) = O(\varepsilon^{-1})$, a typical value for first order methods. Higher order methods generally require $N(\varepsilon) = \varepsilon^{-\alpha}$, $0 \leq \alpha < 1$. The following derivation is not on a standard numerical analysis form but gives a transparent direct estimate of the complexity. Consider the Euler approximation u_n of the complex valued solution u to the ordinary differential equation ($u_n \approx u(x_n)$),

$$\begin{aligned} \frac{\mathrm{d}u}{\mathrm{d}t} &= (2\pi\mathrm{i}/\varepsilon)u\ , \quad u(0) = u_0 \quad |u_0| = 1\ , \quad 0 < x \leq 1\ , \\ u_{j+1} &= u_j + (2\pi\mathrm{i}\Delta x/\varepsilon)u_j\ , \quad x_j = j\Delta x\ , \quad j = 0, 1, \dots, J\ . \end{aligned} \tag{4}$$

The error tolerance δ applied at $x = 1$ implies an upper bound on Δx and thus a lower bound on $N(\varepsilon)$,

$$\begin{aligned} \delta = |u(x_J) - u_J| &= \left|\mathrm{e}^{2\pi\mathrm{i}J\Delta x/\varepsilon} - (1 + 2\pi\mathrm{i}\Delta x/\varepsilon)^J\right| |u_0| \\ &= \left|1 - \left(\mathrm{e}^{-2\pi\mathrm{i}\Delta x/\varepsilon}(1 + 2\pi\mathrm{i}\Delta x/\varepsilon)\right)^J\right| \\ &= \left|1 - \left(1 + 2(\pi\Delta x/\varepsilon)^2 + O((\Delta x/\varepsilon)^3)\right)^J\right|\ , \end{aligned}$$

hence

$$\left(1 + 2(\pi\Delta x/\varepsilon)^2 + O((\Delta x/\varepsilon)^3)\right)^J = 1 + \delta$$

and consequently

$$J \log\left(1 + 2(\pi\Delta x/\varepsilon)^2 + O((\Delta x/\varepsilon)^3)\right) = \log(1 + \delta)\ .$$

With $\delta > 0$ fixed, $J = O((\varepsilon/\Delta x)^2)$ from above and with $N(\varepsilon) = J\varepsilon$, $J = \Delta x^{-1}$ we have $N(\varepsilon) = O(\varepsilon^{-1})$.

2.2 Representation of Functions

The Shannon sampling theorem, quoted above, tells us how much data is needed to fully represent a band-limited function. If it is given by its values on a uniform grid we need at least $2\varepsilon^{-1}$ data points per unit length if ε is the minimal wavelength corresponding to the highest frequency. For serious multi-scale problems the number of unknowns just to represent a function is prohibitively large. We will see below that many modern computational methods exploit special features of the multi-scale problems as for example scale separation. Below is a simple but illustrative argument for the possible reduction in the number of data points needed in the representation of function with scale separation.

Consider a multi-scale function $f_\varepsilon(x) = f(x, x/\varepsilon) = f(x, y)$ of the form (1) that is band limited in both variables x and y. We shall also assume it is 1–periodic in both variables with $\varepsilon = 1/L_1$ and L_1 a positive integer,

$$f(x, y) = \sum_{n=0}^{N} \sum_{m=0}^{M} f_{n,m} \exp\left(2\pi\mathrm{i}(nx + my)\right)\ .$$

If we only knew that $f_\varepsilon(x) = f(x, x/\varepsilon)$, as a function of x was band limited with a uniform grid spacing, Δx, we need $\Delta x < 1/(N + M/\varepsilon)$ in order to guarantee that f_ε can be determined. This means that without the knowledge of the special structure of $f_\varepsilon(x)$ giving scale separation into $O(1)$ and $O(\varepsilon)$ scales we need to resolve the function everywhere on the ε–scale. With the knowledge of scale separation we can reduce the number of data points to $O(1)$ instead of $O(\varepsilon^{-1})$. In both cases the constants in the order estimate depend on M and N.

Let us cluster the data points for which we know f_ε in groups with $\Delta x = 1/L_2$, L_2 and L_1/L_2 positive integers in order to fit with the periodicity assumptions,

$$x_{j,k} = j\Delta x + k\delta x \ , \quad j = 1, \ldots, J \ , \quad k = 1, \ldots, K \ , \quad (\delta x \ll \Delta x) \ .$$

We will show that the set of equations,

$$\sum_{n=0}^{N} \sum_{m=0}^{M} f_{n,m} \exp(2\pi\mathrm{i}(n x_{j,k} + m x_{j,k}/\varepsilon)) = f_\varepsilon(x_{j,k}) \ , \qquad \begin{array}{l} j = 1, \ldots, J \\ k = 1, \ldots, K \end{array} \tag{5}$$

have a unique solution if $J > N$, $K > M$, when $\delta x < \varepsilon/M$ and $\Delta x < 1/N$. With $J = N + 1$ and $K = M + 1$ the coefficients in the system (5) form an $(N + 1)(M + 1)$ by $(N + 1)(M + 1)$ matrix

$$\begin{aligned} A &= \Big(\exp\big(2\pi\mathrm{i}(n x_{j,k} + m x_{j,k}/\varepsilon)\big) \Big) \\ &= \Big(\exp\big(2\pi\mathrm{i}(nj\Delta x + nk\delta x + mj\Delta x/\varepsilon + mk\delta x/\varepsilon)\big) \Big) \\ &= \Big(\exp\big(2\pi\mathrm{i}nj\Delta x\big)\big(1 + O(\varepsilon)\big) \exp\big(2\pi\mathrm{i}mjL_1/L_2\big) \exp\big(2\pi\mathrm{i}mk\delta x/\varepsilon\big) \Big) \\ &= \Big(\big(\mathrm{e}^{2\pi\mathrm{i}\Delta x}\big)^{nj} \Big) \otimes \Big(\big(\mathrm{e}^{2\pi\mathrm{i}\delta x/\varepsilon}\big)^{mk} \Big) + O(\varepsilon) = A_\Delta \otimes A_\delta + O(\varepsilon) \ , \end{aligned}$$

where $A\bar{f} = \bar{f}_\varepsilon$, $\bar{f} = (f_{0,0}, \ldots, f_{J,K})^T$ and $\bar{f}_\varepsilon = (f_\varepsilon(x_{1,1}), \ldots, f_\varepsilon(x_{N,M}))^T$. This matrix A is a tensor product of two Vandermonde matrices plus a matrix the norm of which $\to 0$ as $\varepsilon \to 0$ for given N and M. The matrices A_Δ and A_δ are nonsingular if the inequalities of δx and Δx above are satisfied and A is thus non-singular for ε small enough. There is a unique solution for $J = N+1$, $K + M + 1$ and the same solution is still valid for larger values of N, M that result in over determined systems.

3 Background

The new classes of multi-scale methods signal an important emerging phase in computational science. Let us briefly look back at the earlier development to see how it fits in.

Before the era of computers and in the early days of the computers it was necessary to perform most computational problem analytically. The problem needed a clean mathematical form and an analytic solution, for example, in closed form or in terms of tabulated functions. The computational complexity was minimal.

The improvement in computers, starting in the late 1940s, changed this structure. Not only could computations be made much faster and more accurately, it was not necessary to have an analytic solution. The problem could be discretized directly by, for example, replacing an integral by a Riemann sum or by other quadrature methods. Differential equations were replaced by finite difference or finite element methods. This was a clear paradigm shift and it gave rise to a second phase, a golden era for numerical theory and practice. Moderate size multi-scale problems could be handled.

The theoretical foundation for stability and convergence was developed as symbolized by the Lax equivalence theorem. This was a central factor for the 2005 Abel Prize. The type of mathematics that was needed changed from interpolation techniques, special function theory and asymptotic methods to richer part of analysis including a priory estimates and compactness arguments.

Some of the numerical algorithms that are used today were developed before this period and carry the names of scientists like Newton and Gauss. Most current methods were, however developed during this period. Examples are the following methods: conjugate gradient, QR, singular value decomposition, linear programming, multi-grid, multi-pole, the Fast Fourier Transform (FFT) and finite elements.

For all these methods it was, however necessary to have access to an effective equation that described the solution within a limited range of scales. In the third phase, the one that is now emerging, different scales and different physical processes can be coupled in the same computer simulation. Fundamental physical principles can now be the basis for practical engineering applications. A necessary condition for this development is the present capacity of computers but we also need new computational methods as in the earlier paradigm shift. A new set of mathematical tools are becoming important in the analysis of this approach that includes stochastic processes and statistical mechanics.

4 Numerical Multi-scale Methods

In the classical numerical multi-scale methods the goal is to have a computational complexity of the order of the number of unknowns, i.e. $r = 1$ in (3). The overall complexity will never be less than $O(\varepsilon^{-d})$ and the methods are thus practical only for moderate ranges of scales.

These numerical multi-scale methods that have been invented during the last few decades have been highly successful. Multi-grid, the fast multi-pole method and hierarchical domain decomposition have been able to reduce the computational complexity to the order of the number of unknowns or close to that for important classes of problems [4], [9]. The applications include systems of linear equations originating from realistic differential and integral equations. The algorithms in their original form rely on properties of the solution operator related to scales in order to achieve their optimal computational complexity. This is where the multi-scale features of the algorithms enter. The solution at a point or value in an array might be sensitive to high frequencies in the data nearby and not as sensitive to higher frequencies that originate from far away. This is the property of Calderon–Zygmund operators. The target problems of many of these methods were elliptic partial differential equations.

Other methods in this class are the FFT and the conjugate gradient (CG) method. The mechanisms that make these latter techniques efficient are somewhat different from the earlier ones. The FFT relies on trigonometric identities and the CG method accelerates convergence in the solution of linear systems of equations if the eigenvalues are clustered. The clustering of eigenvalues often corresponds to clustering of scales.

Wavelet based methods can be seen as techniques of this class. In Beylkin, Coifman and Rokhlin [3] it is proved that Calderon–Zygmund operators can be represented by a sparse matrix with a high degree of accuracy. If this representation is combined with an iterative method that converges to a predetermined accuracy in a finite number of iterations we have an optimal method with the exponent $r = 1$.

The wavelet methods also indicate a way for the new class of techniques described in the next section. We are then talking about methods for which some sort of sampling of the unknowns are necessary in order to reduce their number. A thresholded wavelet expansion can be such a representation, which we symbolically can write,

$$f(x) = \sum_{j,k} \hat{f}_{j,k}\psi_{j,k}(x) \approx \sum_{j,k \in I} \hat{f}_{j,k}\psi_{j,k}(x) \ ,$$

where I is the index set corresponding to $|\hat{f}_{j,k}| \geq \delta$, and δ is an error threshold.

5 Current Multi-scale Modeling

We have seen that even with the fastest computers and the fastest standard numerical methods it is not possible to accurately approximate serious multi-scale problems. We can no longer expect to resolve the finest scales all over the space and time domains. A new class of computational methods is aiming at reducing the total number of unknowns in a simulation by using properties like scale separation.

In the simplest case, called type A in [6], the micro-scale is confined to a small part of the computational domain, compare (2) above. A typical application could be crack propagation. Linear elasticity might be a good model for most of the domain but a micro-scale atomistic model may be required to describe the details at the crack tip. The challenge is to couple these two models with appropriate boundary conditions.

In type B problems the micro-scale exists everywhere and influences the macro-scale. Densely distributed local micro-scale simulations are a possibility. This form of sampling of the micro-scale is the basis for the quasicontinuum method, [14]. It is also the basis for the heterogeneous multi-scale method, [6], [7], described below and the so-called equation free method by Kevrekides and collaborators, [12].

5.1 The Heterogeneous Multi-scale Method (HMM)

The HMM is a framework for this new class of multi-scale and often also multi-physics methods. It is a framework for both analysis and for the development of new algorithms. The basic idea is to use as much knowledge as possible of the macro-scale model and then use a micro-scale model to supply the missing data.

The general setting can be presented schematically as follows. We are given a micro-scale system f with state variable u that is assumed to be accurate but too detailed and computationally costly for a full simulation,

$$f(u, d) = 0 \ .$$

The data d is a set of auxiliary conditions as, for example, initial and boundary conditions. Here we are not primarily interested in the microscopic details of u, but rather the macroscopic state of the system, which we denote by U. The macro-scale variable U satisfies some abstract macroscopic equation,

$$F(U, D) = 0 \ ,$$

where $D = D(u)$ stands for the data that is missing in the system and that will be supplied by the micro-scale model. Even if we do not have the ideal situation of an effective equation for U we can use the structure of such an equation, for example, a conservation form. The auxiliary conditions or constraints d depends on the macroscopic state, $d = d(U)$ and we get a coupled self consistent system,

$$\begin{aligned} F(U, D(u)) &= 0 \ , \\ f(u, d(U)) &= 0 \ . \end{aligned}$$

After discretization, for example by a finite difference or finite element methods we have the symbolic algorithm,

$$F_\Delta\big(U_\Delta, D_\Delta(u_\delta)\big) = 0 \ , \tag{6}$$

$$f_\delta\big(u_\delta, d_\delta(U_\Delta)\big) = 0 \ . \tag{7}$$

This can be compactly be formulated,

$$F_\Delta\big(U_\Delta, \tilde{D}_\Delta(U_\Delta)\big) = 0 \ . \tag{8}$$

In convergence proofs the HMM (8) is compared to an effective equation,

$$F_\Delta\big(\bar{U}_\Delta, \bar{D}_\Delta(\bar{U}_\Delta)\big) = 0 \; . \tag{9}$$

The structure but not the details of this equation is needed. The proofs are based on the numerical stability of (9), which implies a bounded inverse and application of an implicit function theorem, [6]. The resulting error estimate takes the form,

$$\|U_\Delta - \bar{U}_\Delta\| \leq C\big(\Delta x^p + e(\mathrm{HMM})\big) \; .$$

The constant C depends on the stability properties and the exponent p is the numerical order of the methods (8) and (9). The term $e(\mathrm{HMM})$ is the error in the data estimation. Here it means the difference between $\bar{D}_\Delta$ and $\tilde{D}_\Delta$ for an appropriate class of U_Δ. This latter type of estimate is not standard in numerical analysis and other fields of mathematics are required. The norm above must be chosen depending on application.

In a typical application (6) may be a finite difference or finite volume method for the Navier–Stokes equations but with no explicit formula for the flux. Instead of an empirical flux formula the flux data will be simulated by a local molecular dynamics computation (7) at every macro grid cell. See [6] for more examples.

5.2 Faster than FFT

We mentioned the fast Fourier transform as an example of a multi-scale method in Sect. 4. The computational complexity with N components is $O(N \log N)$. In order to do better we cannot expect to determine all Fourier modes. If we have an input vector of N values and only need the M largest discrete Fourier components to a given error tolerance δ with probability $1-\delta$, there is a very recent algorithm with complexity $O(\mathrm{poly}(M \log N))$, [11]. We have for simplicity used the same quantifier for both the error estimate and the probability and "poly" stands for "polynomial in". The algorithm requires that these M modes are dominant and much larger than the rest of the Fourier modes. Not all N function values can be involved in the computation and we have again the situation where sampling is required.

The strategy is briefly to first redistribute the M larger modes such that they are not clustered. This is done by a mapping of the independent variables similarly to what is done in random number generators, [10], [11]. After this step the full spectral interval $0 \leq \omega \leq N-1$, $\omega \in \mathbb{Z}$, is divided into I sub-intervals of the same length, Ω_k, $k = 1, \ldots, I$. The norms $\|K_k * f\|_{L_2}$ are then estimated by Monte Carlo simulations. The kernel in the convolution corresponds to a band pass filter for Ω_k, $\hat{K}(\omega)$ is the characteristic function of Ω_k. This process will locate the modes within the appropriate Ω_k with the prescribed probability. A further hierarchical decomposition of those Ω_k containing Fourier modes will locate them to given accuracy in $O(\mathrm{poly}(M \log N))$ operations.

We can actually do better than the above algorithm and reduce the complexity to $O(M)$ by the following new algorithm. The other conditions are the same but the gap between the M largest values and the rest of the Fourier components should be even larger than above. In order to be practical the algorithm must be improved but it is of interest to know where the limit of computational complexity is.

Assume $f(x) = \sum_{j\in J} a_j \exp(2\pi \mathrm{i}\omega_j x)$, $0 < a \leq |a_j| \leq A$, where J is and index set of M integers $0 \leq j \leq N-1$. The function f is known for the integers values $1 \leq x \leq N$.

Let $Q(g)$ be a Monte Carlo estimator of the integral expression for the discrete L_2 norm of g. With f of bounded variance it is well known that with a finite number of evaluation of f we have, [10],

$$\big| \|f\|_{L_2} - Q(f) \big| \leq \delta \; , \qquad \text{with probability} \geq 1-\delta,\ \delta > 0 \; .$$

Define $\bar{\omega} = [\tilde{\omega}+1/2]$, $\tilde{\omega} = \log(Q(K*f)/Q(f))$. The bracket denotes the integer part and K is the inverse discrete Fourier transform of $\hat{K}(\omega) = \mathrm{e}^{\omega}$.

Decompose the spectral domain into three parts,

$$\begin{aligned} \Omega_- &= \{\omega, \omega < \bar{\omega}\} \; , \\ \Omega_0 &= \{\omega, \omega = \bar{\omega}\} \; , \\ \Omega_+ &= \{\omega, \omega > \bar{\omega}\} \; . \end{aligned} \tag{10}$$

If the Monte Carlo estimate is exact and $M = 1$ then $Q(K*f) = \exp(\omega_1)|a_1|$, $Q(f) = |a_1|$ and $\bar{\omega} = \omega_1$. The set Ω_0 will consist of the correct frequency ω_1, the sets Ω_-, Ω_+ will be empty and the coefficient a_1 can be determined arbitrary well by a Monte Carlo approximation of the inner product,

$$a_1 = \frac{1}{N} \sum_{j=1}^{N} f(j) \exp(2\pi \mathrm{i}\omega_1 j) \approx \frac{1}{s} \sum_{j\in S}^{N} f(j) \exp(2\pi \mathrm{i}\omega_1 j) \; ,$$

where S is a random set of s integers, $1 \leq j \leq N$.

If $M > 1$ then

$$Q(K*f) = \sqrt{\sum_{j\in J} \exp(2\omega j)|a_j|^2} \; , \qquad Q(f) = \sqrt{\sum_{j\in J} |a_j|^2}$$

and

$$\min_{j\in J} \omega_j < \tilde{\omega} < \max_{j\in J} \omega_j \; .$$

At most one of the sets in (10) will be empty. The maximum number of elements in Ω_- or Ω_+ is strictly less than M. The procedure can now be repeated in the subsets Ω_- and Ω_+ until $M = 1$. When the procedure continues in the subsets the argument in the Q–estimator should be convolved with the appropriate band pass filter.

It remains to analyze the impact of the error in the Monte Carlo estimate. In the $M = 1$ case the error in $\tilde{\omega}$ with a finite sample can be bounded by $C\delta$ based on bounds of the variances of $K * f$ and f,

$$\big|\|K * f\| - Q(K * f)\big| \le C_1 \mathrm{e}^{\omega_1}\delta \,, \qquad \big|\|f\| - Q(f)\big| \le C_2\delta \,,$$

with probability larger than $1 - \delta$. This implies,

$$\tilde{\omega} = \log\big(\|K * f\|/\|f\| + O(\mathrm{e}^{\omega_1}\delta)\big) \,, \qquad |\omega_1 - \tilde{\omega}| \le C\delta \,.$$

The effect of the error in the case $M > 1$ can be analyzed similarly.

The algorithm does not change if there are other than the M large modes present. Their corresponding amplitudes must, however, be extremely small not to invalidate the error estimates. The details of the algorithm and the error estimates will be given elsewhere.

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Mass in Quantum Yang–Mills Theory (Comment on a Clay Millennium Problem)

L. D. Faddeev

St. Petersburg Department of Steklov Mathematical Institute, St. Petersburg, Russia faddeev@pdmi.ras.ru

Summary. Among seven problems, proposed for the XXI century by the Clay Mathematical Institute [1], there are two stemming from physics. One of them is called "Yang–Mills Existence and Mass Gap". The detailed statement of the problem, written by A. Jaffe and E. Witten [2], gives both motivation and exposition of related mathematical results, known until now. Having some experience in the matter, I decided to complement their text by my own personal comments[1] aimed mostly to mathematical audience.

1 What is the Yang–Mills Field?

The Yang–Mills field bears the name of the authors of the famous paper [4], in which it was introduced into physics. From a mathematical point of view it is a connection in a fiber bundle with compact group G as a structure group. We shall treat the case when the corresponding principal bundle E is trivial

$$E = M_4 \times G$$

and the base M_4 is a four-dimensional Minkowski space.

In our setting it is convenient to describe the Yang–Mills field as a one-form A on M_4 with the values in the Lie algebra $\mathfrak{G}$ of G:

$$A(x) = A^a_\mu(x) t^a \mathrm{d}x^\mu \ .$$

Here x^μ, $\mu = 0, 1, 2, 3$ are coordinates on M_4; t^a, $a = 1, \ldots, \dim G$ – basis of generators of $\mathfrak{G}$ and we use the traditional convention of taking sum over indices entering twice.

Local rotation of the frame

$$t^a \to h(x) t^a h^{-1}(x) \ ,$$

[1] The first variant was published in [3]. In this new version more details are given in the description of renormalization.

where $h(x)$ is a function on M_4 with the values in G induces the transformation of the A (gauge transformation)

$$A(x) \to h^{-1}(x)A(x)h(x) + h^{-1}\mathrm{d}h(x) = A^h(x) \ .$$

The important equivalence principle states that a physical configuration is not a given field A, but rather a class of gauge equivalent fields. This principle essentially uniquely defines the dynamics of the Yang–Mills field.

Indeed, the action functional, leading to the equation of motion via the variational principle, must be gauge invariant. Only one local functional of second order in derivatives of A can be constructed.

For that we introduce the curvature – a two-form with values in $\mathfrak{G}$

$$F = \mathrm{d}A + A^2 \ ,$$

where the second term in the RHS is the exterior product of a one-form and a commutator in $\mathfrak{G}$. In more detail

$$F = F^a_{\mu\nu} t^a \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu \ ,$$

where

$$F^a_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + f^{abc} A^b_\mu A^c_\nu$$

and f^{abc} are structure constants of $\mathfrak{G}$ entering the basic commutation relation

$$[t^a, t^b] = f^{abc} t^c \ .$$

The gauge transformation of F is homogenous

$$F \to h^{-1} F h \ ,$$

so that the 4–form

$$\mathcal{A} = \mathrm{tr}\, F \wedge F^* = F^a_{\mu\nu} F^a_{\mu\nu} \mathrm{d}^4 x$$

is gauge invariant. Here F^* is a Hodge–dual to F with respect to the Minkowskian metric and d^4x is corresponding volume element. It is clear that S contains the derivatives of A at most in second order. The integral

$$\mathcal{S} = \frac{1}{4g^2} \int_{M_4} \mathcal{A} \tag{1}$$

can be taken as an action functional. The positive constant g^2 in front of the integral is a dimensionless parameter which is called a coupling constant. Let us stress that it is dimensionless only in the case of four-dimensional space–time.

Recall that the dimension of a physical quantity is in general a product of powers of three fundamental dimensions – length [L], time [T] and mass [M], with usual units of cm, sec and gr, respectively. However, in relativistic quantum physics we have two fundamental constants – the velocity of light c

and the Planck constant $\hbar$ and we use the convention that $c = 1$ and $\hbar = 1$, reducing the possible dimensions to the powers of length [L]. The Yang–Mills field has dimension $[A] = [\mathrm{L}]^{-1}$, the curvature $[F] = [\mathrm{L}]^{-2}$, the volume element $[\mathrm{d}^4 x] = [\mathrm{L}]^4$, so that an integral in $\mathcal{S}$ is dimensionless. Now, all of $\mathcal{S}$ should be dimensionless, as it has the same dimension as $\hbar$, thus g^2 has dimension zero.

We see that $\mathcal{S}$ contains terms in powers of A of degrees two, three and four

$$\mathcal{S} = \mathcal{S}_2 + \mathcal{S}_3 + \mathcal{S}_4 \ ,$$

which means that the Yang–Mills field is self-interacting.

Among many approaches to quantizing the Yang–Mills theory the most natural is that of the functional integral. Indeed, the equivalence principle is taken into account in this approach by integrating over classes of equivalent fields, so we shall use this approach in what follows. There is no place here to describe in detail this purely heuristic method of quantization, moreover it will hardly lead to a solution of the Clay Problem. However, it will be very useful for an intuitive explanation of this problem, which we shall do here.

2 What is Mass?

It was the advent of special relativity which lead to a natural definition of mass. A free massive particle has the following expression of the energy ω in terms of its momentum p

$$\omega(p) = \sqrt{p^2 + m^2} \ ,$$

where m is called mass. In the quantum version mass appears as a parameter (one out of two) of the irreducible representation of the Poincaré group (the group of motion of the Minkowski space).

In quantum field theory this representation (insofar as m) defines a one-particle space of states $\mathcal{H}_m$ for a particular particle entering the full spectrum of particles. The state vectors in such a space can be described as functions $\psi(p)$ of momentum p and $\omega(p)$ defines the energy operator.

The full space of states has the structure

$$\mathcal{H} = \mathbb{C} \oplus \left(\sum_i \oplus \mathcal{H}_{m_i} \right) \oplus \cdots \ ,$$

where the one-dimensional space $\mathbb{C}$ corresponds to the vacuum state and $\cdots$ means spaces of many-particles states, being tensor products of one-particle spaces. In particular, if all particles in the system are massive the energy has zero eigenvalue corresponding to vacuum and then positive continuous spectrum from $\min m_k$ to infinity. In other words, the least mass defines the gap in the spectrum. The Clay problem requires the proof of such a gap for the Yang–Mills theory.

We see an immediate difficulty. In our units m has dimension $[m] = [\mathrm{L}]^{-1}$, but in the formulation of the classical Yang–Mills theory no dimensional parameter entered. On the other hand, the Clay Problem requires that in the quantum version such parameter must appear. How come?

I decided to write these comments exactly for the explanation how quantization can lead to the appearance of the dimensional parameter when classical theory does not have it. This possibility is connected with the fact that quantization of the interacting relativistic field theories leads to infinities – appearance of the divergent integrals which are dealt with by the process of renormalization. Traditionally these infinities were considered as a plague of the Quantum Field Theory. One can find very strong words denouncing them, belonging to the great figures of several generations, such as Dirac, Feynmann and others. However I shall try to show that the infinities in the Yang–Mills theory are beneficial – they lead to the appearance of the dimensional parameter after the quantization of this theory.

This point of view was already emphasized by R. Jackiw [5] but to my knowledge it is not shared yet by other specialists.

Sidney Coleman [6] coined the name "dimensional transmutation" for this phenomenon, which I am now going to describe. Let us see what all this means.

3 Dimensional Transmutation

The most direct way to introduce the functional integral is to consider the generating functional for the scattering operator. This functional depends on the initial and final configuration of fields, defined by the appropriate asymptotic condition. In a naive formulation these asymptotic configurations are given as solutions A_{in} and A_{out} of the linearized classical equations of motion. Through these solutions the particle interpretation is introduced via well defined quantization of the free fields. However, the more thorough approach leads to the corrections, which take into account the self-interaction of particles. We shall see below how it is realized in some consistent way.

Very formally, the generating functional $W(A_{\mathrm{in}}, A_{\mathrm{out}})$ is introduced as follows

$$\mathrm{e}^{\mathrm{i}W(A_{\mathrm{in}},A_{\mathrm{out}})} = \int_{A \to \substack{A_{\mathrm{in}},\, t\to-\infty \\ A_{\mathrm{out}},\, t\to+\infty}} \mathrm{e}^{\mathrm{i}S(A)} \mathrm{d}A \,, \tag{2}$$

where $S(A)$ is the classical action (1). The symbol $\mathrm{d}A$ denotes the integration and we shall make it more explicit momentarily.

The only functional integral one can deal with is a Gaussian. To reduce (2) to this form and, in particular, to identify the corresponding quadratic form we make a shift of the integration variable

$$A = B + ga \,,$$

where the external variable B should take into account the asymptotic boundary conditions and the new integration variable a has zero incoming and outgoing components.

We can consider both A and B as connections, then a will have only homogeneous gauge transformation

$$a(x) \to h^{-1}(x)ah(x) .$$

However, for fixed B the transformation law for a is nonhomogeneous

$$a \to a^h = \frac{1}{g}(A^h - B) . \tag{3}$$

Thus the functional $S(B+a) - S(B)$ is constant along such "gauge orbits". Integration over a is to take this into account. We shall denote $W(A_{\text{in}}, A_{\text{out}})$ as $W(B)$, keeping in mind that B is defined by A_{in}, A_{out} via some differential equation. Here is the answer detailing the formula (2)

$$\begin{aligned} \mathrm{e}^{\mathrm{i}W(B)} = \mathrm{e}^{\mathrm{i}S(B)} \int \exp \mathrm{i} \left\{ S(B+a) - S(B) + \int \frac{1}{2} \operatorname{tr}(\nabla_\mu a_\mu)^2 \mathrm{d}x \right\} \\ \times \det\bigl((\nabla_\mu + g a_\mu)\nabla_\mu\bigr) \prod_x \mathrm{d}a(x) . \end{aligned} \tag{4}$$

Here we integrate over all variables $a(x)$, considered as independent coordinates. Furthermore, ∇_μ is a covariant derivative with respect to connection B

$$\nabla_\mu = \partial_\mu + B_\mu .$$

The quadratic form $\frac{1}{2}\int(\nabla_\mu a_\mu)^2 \mathrm{d}x$ regularizes the integration along the gauge orbits (3) and the determinant provides the appropriate normalization. This normalization was first realized by V. Popov and me [7] with additional clarification by 't Hooft [8]. I refer to the physical literature [9], [10] for all explanations. One more trick consists in writing the determinant in terms of the functional integral

$$\det(\nabla_\mu + g a_\mu)\nabla_\mu = \int \exp \mathrm{i}\Bigl\{\int \operatorname{tr}\bigl((\nabla_\mu + g a_\mu)\bar{c}\nabla_\mu c\bigr)\mathrm{d}x\Bigr\} \prod_x \mathrm{d}\bar{c}(x)\mathrm{d}c(x)$$

over the Grassman algebra with generators $\bar{c}(x)$, $c(x)$ in the sense of Berezin [11]. These anticommuting field variables play only accessory role, there are no physical degrees of freedom corresponding to them.

The resulting functional which we should integrate over $a(x)$, $\bar{c}(x)$, $c(x)$ assumes the form

$$\begin{aligned} \exp \mathrm{i}\Bigl\{ \frac{1}{2}(M_1 a, a) + (M_0 \bar{c}, c) + \frac{1}{g}\varGamma_1(a) \\ + g\varGamma_3(a,a,a) + g^2\varGamma_4(a,a,a,a) + g\varOmega_3(\bar{c}, c, a) \Bigr\} , \end{aligned} \tag{5}$$

where we use short notations for the corresponding linear, quadratic, cubic and quartic forms in variables a and $\bar{c}$, c. The linear form $\Gamma_1(a)$ is defined via the classical equation of motion for the field $B_\mu(x)$

$$\Gamma_1(a) = \int \operatorname{tr}(\nabla_\mu F_{\mu\nu}(x) a_\nu(x))\mathrm{d}x \, , \tag{6}$$

the forms Γ_3, Γ_4 and Ω_3 are given by

$$\Gamma_3 = \int \operatorname{tr} \nabla_\mu a_\nu [a_\mu, a_\nu] \mathrm{d}x \, , \tag{7}$$

$$\Gamma_4 = \frac{1}{4} \int \operatorname{tr}\big([a_\mu, a_\nu]\big)^2 \mathrm{d}x \, , \tag{8}$$

$$\Omega_3 = \int \operatorname{tr} \nabla_\mu \bar{c} [a_\mu, c] \mathrm{d}x \tag{9}$$

and the operators M_1 and M_0 of the quadratic forms look like

$$M_1 = -\nabla_\rho^2 \delta_{\mu\nu} - 2[F_{\mu\nu}, \cdot] \, , \tag{10}$$

$$M_0 = -\nabla_\rho^2 \, . \tag{11}$$

The equation on the external field B in the naive approach would be the classical equation of motion, assuring that $\Gamma_1(a)$ vanishes. This would correspond to the stationary phase method. However, we shall make a different choice taking into account the appropriate quantum corrections.

It is instructive to use the simple pictures (Feynman diagrams) to visualize the objects (6)–(9). For the forms Γ_1, Γ_3, Γ_4 and Ω_3 they look as vertices with external lines, the number of which equals the number of fields $a(x)$, $\bar{c}(x)$, $c(x)$

(12)

Γ_1 Γ_3 Γ_4 Ω_3

The Green functions G_1 and G_0 for operators M_1 and M_0 are depicted as simple lines

(13)

G_1 G_0

Each end of the lines in (12) and (13) bears indices x, μ, a or x, a characterizing the fields $a_\mu^a(x)$ and $\bar{c}^a(x)$, $c^b(x)$. The arrow on line - ->- - distinguishes the fields $\bar{c}$ and c. Note, that Green functions are well defined due to homogeneous boundary conditions for $a(x)$, $\bar{c}(x)$, $c(x)$.

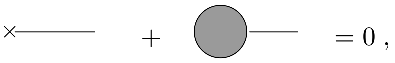
Now simple combinatorics for the Gaussian integral which we get from (4) expanding the exponent containing vertices in a formal series, gives the following answer

$$\exp \mathrm{i}W(B) = \exp \mathrm{i}S(B)(\det M_1)^{-1/2} \det M_0 \times \exp\{\textstyle\sum \text{connected closed graphs}\}\,, \tag{14}$$

where we get a graph by saturating the ends of vertices by lines, corresponding to the Green functions. The term "closed" means that a graph has no external lines.

We shall distinguish weakly and strongly connected graphs. A weakly connected graph can be made disconnected by crossing one line. (In physical literature the term "one particle reducible" is used for such graph.)

The quantum equation of motion, which we impose on B, can be depicted as

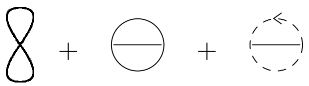


(15)

where the second term in the LHS is a sum of strongly connected graphs with one external line. In the lowest approximation it looks as follows

With this understanding the expression for $W(B)$ is given by the series in the powers of the coupling constant g^2

$$W(B) = \frac{1}{g^2}\int \mathrm{tr}(F \wedge F^*) + \ln\det M_0 - \frac{1}{2}\ln\det M_1$$

$+ g^2($  $)$

$$+ \sum_{k=3}^{\infty} g^{2(k-1)}(\text{strongly connected graphs with } k \text{ loops})\,. \tag{16}$$

From now on we use a "Euclidean trick" here, changing x_0 to $\mathrm{i}x_0$, so that M_0 and M_1 become elliptic operators. This answer can be considered as an alternative definition of the functional integral (2). Two natural questions can be asked:

1. Are the individual terms in (16) well defined?
2. Does the series converge?

Whereas we know almost nothing about the second question, the answer to the first one is quite instructive. Here we are confronted with the problem of divergences and renormalization.

Let us turn to the zero order in g^2 term in (16). It is given by determinants of operators M_1 and M_0, which clearly diverge and must be regularized. The trivial regularization is the subtraction of an infinite constant, corresponding to the dets for $B = 0$. Then we can use the formula

$$\ln\det M_i(B) - \ln\det M_i(0) = -\int_0^\infty \frac{\mathrm{d}t}{t}\,\mathrm{Tr}\left(\mathrm{e}^{-M_i(B)t} - \mathrm{e}^{-M_i(0)t}\right)\,, \tag{17}$$

where $i = 0, 1$. The Green functions $D_i(x, y; t)$ of the parabolic equations

$$\frac{\mathrm{d}D_i}{\mathrm{d}t} + M_i D_i = 0, \qquad D_i|_{t=0} = I\delta(x-y) \tag{18}$$

has the well known expansion for small t

$$D(x, y; t) = \frac{1}{4\pi^2 t^2} \mathrm{e}^{-\frac{|x-y|^2}{4t}} \left(a_0(x, y) + t a_1(x, y) + t^2 a_2(x, y) + \ldots\right),$$

where the coefficients $a_0, a_1, a_2, \ldots$ are functionals of B. (Recall that we deal with 4–dimensional space–time.) The trace in (17) means

$$\int \operatorname{tr} D(x, x; t) \mathrm{d}x . \tag{19}$$

The coefficient a_0 is the holonomy for connection B along the straight line, connecting points x and y. Clearly $a_0(x, x)$ equals unity and so its contribution disappears from (17) due to the subtraction of $\exp(-M(0)t)$. Now $a_1(x, x)$ for the operator M_0 vanishes and same is true for $\operatorname{tr} a_1(x, x)$ for M_1. So what remains is the contribution of a_2 to (17) which diverges logarithmically in the vicinity of $t = 0$. The expansion is valid for small t, so we divide the integration in (17) as

$$\int_0^\infty = \int_0^\mu + \int_\mu^\infty \tag{20}$$

and regularize the first integral as

$$\begin{aligned} &\int_\epsilon^\mu \frac{\mathrm{d}t}{t} \int \operatorname{tr} a_2(x, x) \mathrm{d}x \\ &\quad + \int_0^\mu \frac{\mathrm{d}t}{t} \int \left(\operatorname{tr} D(x, x; t) - \operatorname{tr} D(x, x; t)|_{B=0} - \operatorname{tr} a_2(x, x) + \mathcal{O}(t^2)\right) \mathrm{d}x . \end{aligned}$$

In this way we explicitly separated the infinite part proportional to $\ln \epsilon/\mu$. (In the physics literature one uses large momentum cutoff Λ instead of short auxiliary time ϵ; the $\ln \epsilon/\mu$ looks like $-2\ln \Lambda/m$, where m has the dimension of mass.)

Now observe that $\int \operatorname{tr} a_2(x, x) \mathrm{d}x$ is proportional to the classical action $\int \operatorname{tr}(F \wedge F^*)$. This follows from general considerations of gauge invariance and dimensionlessness, but can also be found explicitly together with the corresponding numerical coefficient. We get

$$\begin{aligned} W(B) = &\frac{1}{4}\left(\frac{1}{g^2} + \frac{11}{48\pi^2} C(G) \ln \frac{\epsilon}{\mu}\right) \int \operatorname{tr}(F \wedge F^*) \\ &+ \text{finite zero order terms} + \text{higher order loops} . \end{aligned} \tag{21}$$

Here $C(G)$ is a value of a Casimir operator for group G in the adjoint representation.

Now we invoke the idea of renormalization à la Landau and Wilson: the coupling constant g^2 is considered to be a function of the regularizing parameter ϵ in such a way that the coefficient in front of the classical action stay finite when $\epsilon \to 0$

$$\frac{1}{g^2(\epsilon)} + \beta \ln \frac{\epsilon}{\mu} = \frac{1}{g^2_{\mathrm{ren}}} , \qquad \beta = \frac{11}{3} \frac{C}{16\pi^2} . \tag{22}$$

This can be realized only if the coefficient β is positive, which is true in the case of the Yang–Mills theory. Of course $g^2(\epsilon) \to 0$ in this limit.

A similar investigation can be done for the quantum equation of motion (15). The one loop diagrams are divergent, but the infinite term is proportional to the classical equation of motion, so that (15) acquires the form

$$\nabla_\mu F_{\mu\nu} + g^2_{\mathrm{ren}}(\text{finite terms}) = 0 .$$

Higher loops contribute corrections to the renormalization (22), however their influence is not too drastic. I can not explain this here and mention only that it is due to the important general statement, according to which the logarithmic derivative of $g^2(\epsilon)$ over ϵ does not depend on ϵ explicitly

$$\frac{\mathrm{d}g^2(\epsilon)}{\mathrm{d}\ln\epsilon} = \beta\big(g^2(\epsilon)\big) ,$$

where

$$\beta(g) = \beta g^3 + \mathcal{O}(g^5) .$$

This relation is called the renormalization group equation; it follows from it and the requirement that the renormalized charge does not depend on ϵ and that the correction to (22) have form $\ln\ln\epsilon/\mu$ and lower.

We stop here the exposition of the elements of quantum field theory and return to our main question of mass. We have seen that the important feature of the definition of $W(B)$ and the equations of motion was the appearance of the dimensional parameter. Thus the asymptotic states, which characterize the particle spectrum, depend on this parameter and can be associated with massive particles. Let us stress that the divergences are indispensable for this, they lead to the breaking of the scale invariance of the classical theory.

In our reasoning it was very important that divergences have logarithmic character, which is true only for the 4–dimensional space–time. All this and positivity of the coefficients β in (22) distinguishes the Yang–Mills theory as a unique quantum field theory, which has a chance to be mathematically correct.

It is worth to mention that the disenchantment in quantum field theory in the late fifties and sixties of the last century was connected with the problem of the charge renormalization. In the expressions, similar to (22), for all examples, fashionable at that time, the coefficient β was negative. This was especially stressed by Landau after investigation of the most successful example of quantum field theory – quantum electrodynamics. The realization in the beginning of seventies of the fact that in Yang–Mills theory the coefficient β is positive, which is due to 't Hooft, Gross, Wilchek and Politzer, changed the attitude of physicists towards the quantum theory and led to the formulation of Quantum Chromodynamics. (This dramatic history can be found in [12].)

Conclusion

We have seen that the quantization of the Yang–Mills field theory leads to a new feature, which is absent in the classical case. This feature – "dimensional transmutation" – is the trading of the dimensionless parameter g^2 for the dimensional one μ with dimension $[\mathrm{L}]^2$. We have also seen that on a certain level of rigour the quantization procedure is consistent. This gives us hope that the Clay problem is soluble. Of course, the real work begins only now. I believe that a promising direction is the investigation of the quantum equation of motion, which should enable us to find solutions with nontrivial mass. One possibility will be the search for solitonic solutions. Some preliminary formulas in this direction can be found in [13].

I hope, that this text could be stimulating for a mathematician seriously interested in an actual problem of the modern theoretical physics.

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On Scaling Properties of Harmonic Measure

Peter W. Jones

Department of Mathematics, Yale University, New Haven, CT 06520, USA
jones-peter@yale.edu

1 Introduction

This short article gives an exposition of some open problems concerning harmonic measure for domains in Euclidean space. This is an area where Lennart Carleson has been a leading figure for about fifty years. Like many other analysts, this author had his career shaped to a large extent by Lennart, and this provides me an opportunity to both wish him a happy birthday and thank him for all the assistance he has given me for nigh thirty years.

Recall that the *harmonic measure* for a base point $z_0 \in \Omega$ is the (unique) probability measure ω on $\partial\Omega$ so that

$$F(z_0) = \int F(z)\mathrm{d}\omega(z)$$

for all harmonic functions F on Ω that are (modulo small technicalities) continuous up to $\partial\Omega$. Despite decades of intensive research, we are far from understanding the "fine structure" of harmonic measure. Certainly the greatest achievement here is N. Makarov's theorem [11] that on any simply connected planar domain, ω (for any base point) is supported on a set of Hausdorff dimension one, and ω puts no mass on any set of dimension less than one. In modern parlance this is written as $\dim(\omega) = 1$. A related, surprising theorem due to Carleson [5] is that for "square" Cantor sets (as boundary) in the plane, $\dim(\omega) < 1$, no matter how large the dimension of the Cantor set. In $\mathbb{R}^d$, $d \geq 3$, our knowledge is much less complete, though notable results due to Bourgain [4], Wolff [12], and others provide some knowledge of basic scaling laws.

It was understood in the 1990's (see [6]) that dynamical systems and Conformal Field Theory were intimately tied to these problems, at least in dimension two. It is a curious state of affairs that CFT as it is understood today, makes no notable predictions for these problems. This is perhaps even more surprising in light of the great success CFT has had with SLE. Exactly how the full story will unfold remains mysterious. My guess is that we are missing fundamental concepts, and that the future will bring some unsuspected, closer connections between analysis and statistical physics. If the situation is murky for $d = 2$, it is much worse for $d \geq 3$. All results known there are the end products of arguments of real variable type, and therefore cannot yield sharp constants. Whether there can be a unified approach to all dimensions seems now to be an untouchable problem. If we are very lucky, the new generation may give us the solution due to the rise of a young star of Lennart Carleson's caliber and vision.

2 Harmonic Measure in the Plane

We discuss here various conjectures concerning the fine structure of harmonic measure. In the plane one has some extra measure of confidence in these conjectures due to experience from conformal mappings as well as Conformal Field Theory. A guiding principle taken from CFT is that all expressions should be simple and analytic (in the parameter values). We start with some examples from dimension two and then turn to $d \geq 3$ in the following section.

The first conjecture we discuss concerns conformal mappings $h : \mathbb{D} \to \Omega$, where Ω is a bounded domain. (All conjectures are the same for mappings h of $\{|z| > 1\}$ to Ω, where $h(\infty) = \infty$.) Let $t \in \mathbb{C}$ be a complex number and consider the growth of integral means for $|(h')^t|$. Define $\beta_h(t) \geq 0$ to be the smallest real number such that

$$\int_0^{2\pi} |h'(re^{i\theta})^t| d\theta = \mathcal{O}\big((1-r)^{-\beta_h(t)}\big) .$$

Similarly we define the *pressure spectrum*,

$$\beta_{sc}(t) = \sup \beta_h(t) ,$$

where the supremum is taken over all conformal maps h to bounded domains. (The "sc" stands for simply connected.) It is a nontrivial fact (the "snowflake construction") that for every $\varepsilon > 0$ and every t there is an h such that

$$\int_0^{2\pi} |h'(re^{i\theta})^t| d\theta \geq c(1-r)^{\varepsilon - \beta_{sc}(t)}$$

holds for all $r < 1$. (See e.g. [6] for the case $t = 1$.)

The first conjecture we list is

$$\beta_{sc}(t) = |t|^2/4 , \qquad |t| \leq 2 \tag{1a}$$

and

$$\beta_{sc}(t) = |t| - 1 , \qquad |t| \geq 2 . \tag{1b}$$

The phase transition at $|t| = 2$ can be (partially) understood by looking at $t = 2$ and noticing the bound $|h'(r\exp\{\mathrm{i}\theta\})| \leq c(1-r)^{-1}$, which is due to the finite area of the image domain. (Thus (1b) holds for $t \geq 2$.) The conjecture in (1) was introduced by Kraetzer [9], but now carries the slightly ungainly name of the Brennan–Carleson–Jones–Kraetzer Conjecture. (This is because Brennan's Conjecture was for the special value $t = -2$, while Carleson and Jones had made the conjecture for $t = 1$.) Actually, I. Binder's name should be added to the list of names mentioned because he had the idea of introducing complex values of t.

If we restrict to real values of $t \in [-2, 2]$, the conjecture has two equivalent forms. The first of these is in terms of the multifractal formalism, which has the additional feature of adding Beurling's estimate on harmonic measure in a more transparent form. Recall that if ω is a (locally finite) Borel measure, the $f(\alpha)$ *spectrum* is defined by

$$f(\alpha) = \mathrm{Dimension}(E_\alpha)\ ,$$

where we understand the dimension in question to be the Hausdorff dimension and where (without getting too technical)

$$E_\alpha = \big\{z \mid \omega\big(D(z,r)\big) \sim r^\alpha\big\}\ .$$

Here $D(z,r)$ is the disk centered at z and of radius r, and the $\sim$ symbol means that this holds as $r \to 0$. The reformulation of (1) (for $t \geq -2$) is that for ω the harmonic measure on a bounded, simply connected domain,

$$f(\alpha) \leq 2 - 1/\alpha\ . \tag{2}$$

Again, the conjecture implicitly states that the estimate in (2) is optimal. We define as before

$$f_{\mathrm{sc}}(\alpha) = \sup f(\alpha)\ ,$$

where the supremum is now taken over all simply connected domains. (Unlike β_{sc}, the estimates for $f(\alpha)$ do not depend on whether the domain is bounded or not.) Thus the conjecture is

$$f_{\mathrm{sc}}(\alpha) = 2 - 1/\alpha\ , \qquad \alpha \geq 1/2\ . \tag{3}$$

The proof that conjectures (1) and (3) are equivalent involves a stopping time argument followed by a renormalization procedure. The algebra involved yields the relationship

$$t = 2 - 2/\alpha$$

for $\alpha \geq 1/2$. One builds by a snowflake construction a conformal map h where

$$|h'(r\mathrm{e}^{\mathrm{i}\theta})| \leq c(1-r)^{\varepsilon+1-1/\alpha}$$

and where only this maximal growth is used to estimate $\beta_h(t)$. Conversely, given h one estimates $f(\alpha)$ by a similar construction.

This reasoning can be extended to give another (equivalent) formulation for Hölder domains. Recall that a simply connected domain Ω is called a γ *Hölder domain*, $0 < \gamma < 1$, if (any) Riemann map $h : \mathbb{D} \to \Omega$ is in the Hölder space Λ_γ, $|f(z) - f(w)| \leq c|z-w|^\gamma$, $z, w \in \mathbb{D}$ (equivalently $\overline{\mathbb{D}}$). This is the same as $|f'(z)| \leq c'(1-|z|)^{\gamma-1}$. The conjectures (1) and (3) are equivalent (for the appropriate range of t) to the conjecture

$$\Omega \text{ is a } \gamma \text{ Hölder domain} \quad \Longrightarrow \quad \dim(\partial\Omega) \leq 2 - \gamma \,. \tag{4}$$

The algebra used here is the relation $\alpha = 1/\gamma$, and the understanding of (4) is that the estimate $2 - \gamma$ is best possible.

There is yet another formulation that is believed to be equivalent (for the range $t \in [-2, 2]$) in terms of quasiconformal mappings. For a globally quasiconformal map F let k be the bound for the lower dilatation. (So $0 \leq k < 1$ and $k = 0$ if and only if F is conformal.) Let $\beta_k(t)$ be the pressure function where the supremum is taken over all h having a globally quasiconformal extension F with bound k. The conjecture for $t \in [-2, 2]$ is that

$$\beta_k(t) = \beta(kt) \,. \tag{5}$$

Some support for this is given by a remarkable theorem of Smirnov (unpublished), which is one of the few conjectured upper bounds that has been proven. Smirnov's result is that if h has an extension F with bound k, then

$$\dim\big(F(S^1)\big) \leq 1 + k^2 \,.$$

Recall that Beurling's theorem states that for a simply connected domain,

$$\omega\big(D(z,r)\big) \leq c r^{1/2}$$

where c depends only on the inradius of the base point for harmonic measure. Here $D(z, r)$ is the disk centered at z with radius r. A trivial consequence of Beurling's theorem is

$$f_{\mathrm{sc}}(\alpha) = 0 \,, \qquad \alpha < 1/2 \,,$$

because the sets in question are empty.

What is the evidence for conjectures (1), (3) and (4)? First we note that (1) is true for $t \geq 2$. For $t = -2$ this is Brennan's conjecture, which is supposed to correspond to the (Beurling-type) conjecture $f_{\mathrm{sc}}(1/2) = 0$. For $t = 1$ the conjecture is due to Carleson–Jones [6], who also provided some computer evidence. A small surprise there is the tie to coefficient problems for the class Σ of functions univalent on $\{|z| > 1\}$ having Laurent expansion

$$z + \sum_{n=1}^{\infty} b_n z^{-n} \,.$$

Unlike the case for de Brange's theorem ($|a_n| \le n$) for the class S, there seems to be no natural guess for the maximal size of b_n. Instead it is shown that if $B_n = \sup|b_n|$, the supremum being taken over Σ, then

$$\lim_{n\to+\infty} \frac{\log B_n}{\log n} = \gamma_\Sigma$$

exists and (surprise) $\gamma_\Sigma = \beta(1) - 1$. (Thus the conjecture that $\gamma_\Sigma = -3/4$.)

Returning to other evidence, the value $\alpha = 1$, which corresponds to $t = 0$, should be understood as the theorem of Makarov [11]: For any simply connected domain the harmonic measure is supported on a set of (exactly) Hausdorff dimension one. (More precisely, Makarov's theorem tells one that the $|t|^2/4$ conjecture is correct for $t = 0$ in the sense that $\beta_{\mathrm{sc}}(t)$ should be quadratic near $t = 0$.) Another way of rephrasing these results and conjectures is the following list:

$\alpha = 1/2 \;\leftrightarrow\; t = -2 \;\leftrightarrow\;$ Brennan's Conjecture and Beurling's Theorem
$\alpha = 1 \;\leftrightarrow\; t = 0 \;\leftrightarrow\;$ Makarov's Theorem
$\alpha = 2 \;\leftrightarrow\; t = 1 \;\leftrightarrow\;$ Carleson–Jones Conjecture and $\ell(\Gamma_\varepsilon) \sim \varepsilon^{-1/4}$

By the last entry we mean that if Ω is a bounded domain then Γ_ε is the curve $\{z \mid G(z, z_0) = \varepsilon\}$, where G is Green's function for Ω with base point z_0. If we integrate $|h'|$ over $\{G(z, 0) = \varepsilon\}$ on the disk (essentially the circle of radius $1 - \varepsilon$ about the origin). The $|t|^2/4$ conjecture says that the extremal case is the length of Γ_ε (which is exactly the integral of $|h'|$) should be $\mathcal{O}(\varepsilon^{-1/4})$.

The upshot is that for these three special values there is a corresponding "physical" quantity that is either known (Beurling's or Makarov's Theorem) or reasonably conjectured ($t = 1$, $\alpha = 2$). It would be interesting to see if there is a longer list of natural, "physical" values of t, α. (Of course $t = 2$, $\alpha = +\infty$ corresponds to finite area.)

For the $f_{\mathrm{sc}}(\alpha)$ conjecture it should be noted that the asymptotics are correct. By the results of [7], there are constants c_1 and c_2 such that for $\alpha \ge 1$,

$$2 - c_1/\alpha \le f_{\mathrm{sc}}(\alpha) \le 2 - c_2/\alpha\,. \tag{6}$$

Now the study of $f(\alpha)$ is also well defined for general (i.e. non-simply connected) domains in $\mathbb{R}^2$ (as well as in $\mathbb{R}^d$). The results of [7] are actually for general domains, and can be expressed as bounds for the "universal" spectrum:

$$2 - c_1/\alpha \le f_u(\alpha) \le 2 - c_2/\alpha\,, \qquad \alpha \ge 1\,. \tag{7}$$

Here $f_u(\alpha) = \sup f(\alpha)$, the supremum being taken over all planar domains. For general domains in $\mathbb{R}^2$ one cannot have conjecture (3) for $\alpha < 1$, as the correct result there is $f_u(\alpha) = \alpha$. (It pays to use Cantor sets as boundaries.) One might think that by using Cantor sets one could obtain $f_u(\alpha) > f_{\mathrm{sc}}(\alpha)$ at least in the range $\alpha > 1$. (By the theorem of Jones–Wolff [8], $f_u(1) = 1$.) However, this turns out not to be the case. Binder and Jones have announced [2]:

$$f_u(\alpha) = f_{\mathrm{sc}}(\alpha)\ , \qquad \alpha \geq 1\ . \tag{8}$$

As a consequence, the correct conjecture is

$$f_u(\alpha) = 2 - 1/\alpha\ , \qquad \alpha > 1\ , \tag{9}$$

with the value $\alpha = 1$ being a theorem. Note that by (7) the asymptotic behavior is correct. Before discussing (8) let us remark on a general ($d = 2$) philosophy: All such expressions are analytic functions of low complexity. This philosophy is the simple consequence of adopting a CFT point of view. It seems curious that conjectures (1) and (3) do not seem to exactly fit into our present understanding of CFT, even if all arguments (e.g. renormalization) are from the philosophy of CFT. The point here is that the correct universality class of domains does not come from the canonical lists of CFT, which include SLE. Those domains are very far from extremal (for (1) and (3)) because (e.g. $0 < \kappa \leq 4$) the two sides of the SLE trace are statistically the same. One expects the extremal domains for (1) and (3) to be "one sided", i.e. the exterior domain does not have extremal behavior. It is, however, not impossible that CFT could be directly brought to bear on these problems.

The result (8) has a somewhat curious history, and it is unclear if the methodology used is optimal. In any case, the proof is via a two step argument. The first step is to show that if a choice of domain Ω and $\alpha > 0$ are given, then (for $\varepsilon > 0$) there is a polynomial P, with Julia set J, such that

$$f(\alpha, J^c) \geq f(\alpha, \Omega) - \varepsilon\ .$$

The polynomial P has attached to it both good news and bad news. The good news is that P can be assumed to act hyperbolically on its Julia set J. In addition, the Julia set can be chosen to be of *pure Cantor type*, i.e. all critical points are outside of J and in the basin of infinity, $P^n(c) \to \infty$ for all critical points c. (If Ω is simply connected, one can alternatively demand that J is a Jordan curve, and P is hyperbolic on J.) The bad news is that as $\varepsilon \to 0$, the polynomial constructed by [2] has degree tending to infinity. This "bad" behavior is indeed necessary if J is to approximate $\partial\Omega$ in the correct technical sense. Step two in the proof of (8) is to invoke a remarkable result due to Binder–Makarov–Smirnov: If P and J are of pure Cantor type, there is a polynomial Q, degree(Q) = degree(P), such that the Julia set is connected and

$$f(\alpha, A_\infty) \geq f(\alpha, J^c)\ ,$$

where A_∞ is the basin of infinity for Q. It is worth remarking that while this theorem of Binder, Makarov and Smirnov appears to be simply the maximum principle, no elementary proof is known at present. To sum up, to prove (6) one first "approximates" the boundary of Ω by a polynomial Julia set of pure Cantor type, so that $f(\alpha, J^c) \geq f(\alpha, \Omega) - \varepsilon$. Then one applies the result of Binder, Makarov and Smirnov to "homotopy" J^c to the compliment of a connected Julia set $\tilde{J}$. This means that for $\alpha \geq 1$,

$$f_u(\alpha) = f_{\mathrm{dsc}}(\alpha) , \tag{10}$$

where the subscript d stands for (conformal) dynamic. It is indeed remarkable that (10) holds, even if there were early hints in [6] that this would be the case. (There one built a non-conformal dynamical system.)

The boldest form of the conjecture is that for (10) one need not consider high degree polynomials, but may restrict to Julia sets for $z^2 + c$, where c is in the Mandelbrot set. Though the evidence for this is slight, it is positive. If this were indeed true, it would show an unexpected form of universality for quadratic Julia sets. Only slightly stronger is the conjecture that, for all α, the complement of the Mandelbrot set (M) is extremal. This is because if c is a boundary point of M and J is the Julia set for the parameter c, "near c, M looks like J".

It should also be remarked that numerical evidence for conjecture (1) was given by Kraetzer [9]. It seems there is more work to be done here, especially for complex values of t. A very nice idea has been introduced by D. Beliaev [1]. He defines a class of "conformal snowflakes" by using a particular randomization process. He is then able to get rigorous, computer assisted proofs of lower bounds for the pressure function $\beta(t)$.

An amusing aspect of these problems is that it seems likely that the proofs for upper bounds (e.g. $\beta(t) \leq |t|^2/4$, $|t| \leq 2$) will be quite different from those for the corresponding lower bounds. On this point, the only thing that seems evident is that one should take unbounded domains with compact boundaries (of log-capacity one). This is of course also the natural setting for polynomial dynamics.

3 Harmonic Measure in $\mathbb{R}^d$

Our knowledge of harmonic measure and the $f(\alpha)$ spectrum is much less complete in $\mathbb{R}^d$, $d \geq 3$, than for $d = 2$. What we do know corresponds to experience from CFT: Dimension two is special. As an example of this consider the support of Harmonic measure for a domain Ω. In $d = 2$ the results of Makarov and Jones–Wolff show that there is always a set of dimension one that supports harmonic measure and (Makarov) if Ω is simply connected one cannot use a smaller dimension. In other words, $f(\alpha) < \alpha$ for $\alpha > 1$ and for simply connected domains $f(1) = 1$. This means $f(1)$ is given by $\partial\Omega = S^1$. Now for $d \geq 3$ this might lead one to expect that $f(\alpha) < \alpha$ for $\alpha > d-1$, i.e. there is a set of dimension at most $d-1$ that supports harmonic measure (the Øksendal Conjecture). However, Tom Wolff [12] has provided counterexamples (of "snowball-type") showing this is false. On the positive side we know (Bourgain [4]) that harmonic measure is always supported on a set of dimension $\leq d-\varepsilon(d)$. The weakest conjecture that fits known properties for the dimension of the support of harmonic measure is

$$\dim(\omega) \le d - \varepsilon(d) \ , \tag{11}$$

where $\varepsilon(d) \to 0$ as $d \to +\infty$. It is likely that this is relatively easy. As justification for this conjecture one could cite Jones–Makarov [7], where it is shown that in $\mathbb{R}^d$,

$$d - c_1/\alpha^{d-1} \le f_u(\alpha) \le d - c_2/\alpha^{d-1} \ , \tag{12}$$

where c_1 and c_2 are dimension dependent.

One of the reasons that we are presently lacking precise knowledge of $\dim(\omega)$ in $d \ge 3$ is the lack of arguments of complex variables type. A (very) formal attempt to generalize the proof of Jones–Wolff to higher dimensions leads to the conjecture

$$\dim(\omega) \le d - \frac{1}{d-1} \tag{13}$$

because (!) if $\Delta u = 0$ in $\mathbb{R}^d$, then $|\text{gradient}(u)|^p$ is subharmonic for $p \ge (d-2)/(d-1)$. Corresponding to (13) is the statement

$$f_u\Big(d - \frac{1}{d-1}\Big) = d - \frac{1}{d-1}$$

as well as

$$f(\alpha) < \alpha \ , \qquad \alpha > d - \frac{1}{d-1} \ .$$

If one now makes the supposition that $f_u(\alpha) = d - c_d \alpha^{-d+1}$ for large α, one comes to a somewhat reasonable looking formula. We first denote by $\alpha(\omega)$ the (universal) dimension of harmonic measure, so that by conjecture (13), $\alpha(\omega) = d - (d-1)^{-1}$. Algebra then leads one to the possibility

$$f_u(\alpha) = d - \frac{1}{d-1}\left(\frac{\alpha(\omega)}{\alpha}\right)^{d-1} \tag{14}$$

for values $\alpha \ge \alpha(\omega)$. Notice that this has the correct asymptotics as $\alpha \to +\infty$, and has $f_u(\alpha) < \alpha$ for $\alpha > \alpha(\omega)$. If we set $d = 2$ we also recover the conjecture $f_u(\alpha) = 2 - 1/\alpha$, $\alpha \ge 1$. On the other hand we have $f'(\alpha(\omega)) < 1$, which seems unreasonable. If we wish also to make $f'(\alpha(\omega)) = 1$, thus providing for a smoother phase transition, the next and perhaps more reasonable guess is

$$f(\alpha) = d - \frac{1}{d-1}\big(\alpha + 1 - \alpha(\omega)\big)^{1-d} \ , \tag{15}$$

for $\alpha \ge \alpha(\omega)$. Of course, whether one chooses (14) or (15), one should have $f(\alpha) = \alpha$ for $0 \le \alpha \le \alpha(\omega)$. Conjecture (15) has the advantage that f' exists for all α (and $f'(\alpha(\omega)) = 1$). I am unsure whether one can provide any other justification for (14) and (15) beyond the following: They fit all known facts; give us the “correct” conjecture in $d = 2$; are based on “simple” (here rational) functions; and interpolate analytically through dimensions. The interpretation of (14) or (15) for non-integer dimensions is unclear to me.

As is the case for $d = 2$, it seems clear that, whatever the correct answer is for $f_u(\alpha)$, the proofs of upper versus lower bounds will be quite different. An examination of the arguments of [6] and [12] makes it clear that near extremals for $f_u(\alpha)$ can be built from non-conformal dynamical systems. But in $d \geq 3$ there is no natural analogue of Julia sets and/or conformal dynamics, or rather it seems unlikely that this is how one should proceed. Perhaps there are natural dynamical systems in $d \geq 3$ that give rise to the appropriate domain, but it would seem that if this were the case, those dynamical systems are not among the ones we now are aware of. It also seems unlikely that simply connected domains could be useful when $d \geq 3$. This is due to the fact that the potential theory in $d \geq 3$ puts zero capacity on line segments, and consequently $f_u(\alpha) = f_{\mathrm{sc}}(\alpha)$ actually holds for all $\alpha > 0$. (As far as I am aware, no one has written down the proof of this rather elementary statement.)

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The Heritage of Fourier

Jean-Pierre Kahane

Département de mathématiques, Université Paris-Sud Orsay, Bât. 425, F-91405 Orsay Cedex, France jean-pierre.kahane@math.u-psud.fr

1 Purpose of the Article

The heritage of Fourier is many-sided.

First of all Fourier is a physicist and a mathematician. The name Fourier is familiar to mathematicians, physicists, engineers and scientists in general. The Fourier equation, meaning the heat equation, Fourier series, Fourier coefficients, Fourier integrals, Fourier transforms, Fourier analysis, Fast Fourier Transforms, are everyday terms. The Analytical Theory of Heat is recognized as a landmark in science.

But Fourier is known also as an Egyptologist. He wrote an extensive introduction to the series of books entitled "Description de l'Egypte". He was in Egypt when the Rosetta stone was discovered, and Jean-François Champollion, who deciphered the hieroglyphs, was introduced in the subject by Fourier.

He was also an administrator and a politician. He took part in the French Revolution (Arago said that he was a pure product of the French Revolution, because he was supposed first to become a priest), he followed Bonaparte and Monge in Egypt as "secrétaire perpétuel de l'Institut d'Egypte", then Bonaparte elected him as prefect in Grenoble where he led a very important action in health and education, and he became a member of both Académie des sciences and Académie Française when he settled back in Paris after the fall of Napoleon. He was elected as Secrétaire perpétuel de l'Académie des sciences and played a role for the recognition of statistics in France.

His scientific work does not consist only in the analytical theory of heat and the tools that he created for this theory. He was interested in algebraic equations and his work on the localization of the roots is the transition from Descartes to Sturm; unfortunately he neglected Galois. He himself was neglected for his work on inequalities, what he called "Analyse indéterminée". Darboux considered that he gave the subject an exaggerated importance and did not publish the papers on this question in his edition of the scientific works of Fourier. Had they been published, linear programming and convex analysis would be included in the heritage of Fourier.

Fourier was a learned man and a philosopher in the sense of the eighteenth century. In a way he is a late representative of the Age of Enlightenment. On the other hand he is the main reference for Auguste Comte, a starting point for the French "positivism" of the nineteenth century.

I shall concentrate on a narrow but important part of his scientific heritage, namely the expansion of a function into a trigonometric series and the formulas for computing the coefficients. It is a way to enter the way of thinking of Fourier and its relation to physics and natural philosophy, as well as to explore the purely mathematical continuation of his work.

About the way of thinking of Fourier my general theme is that it has been disregarded for a long time, in France if not in Germany, and that it became very popular quite recently. This will be explained by a few facts and quotations.

About the continuation of his work on trigonometric series I shall focus on a very few topics according to their historical and present interest. A good part of the Conference on "Perspectives in Analysis" can be considered as a illustration of the heritage of Fourier.

The main part of the article is made of quotations and comments (2.1 Victor Hugo, 2.2 Jacobi, 2.3 Fourier, 2.4 Dirichlet and Riemann). Section 3 is devoted to the Riemann theory of trigonometric series and Sect. 4 to the convergence problem (4.1 The Carleson Theorem, 4.2 Variations About Convergence). The end, Sect. 5, is about the coming back of Fourier.

2 A Few Quotations

2.1 Victor Hugo

Let me begin with Victor Hugo. In 1862, he was in exile in the island of Guernsey, where he wrote a large part of his work. It is the year when his novel "Les misérables" was published. This novel contains a lot of information on life in France at the beginning of the nineteenth century. One chapter is entitled "1817". Joseph Fourier appears in this chapter with a short sentence:

> Il y avait à l'académie des sciences un Fourier célèbre que la postérité a oublié, et dans je ne sais quel grenier un Fourier obscur dont la postérité se souviendra.
>
> (*Les Misérables*, Victor Hugo 1862)

> There was at the Académie des sciences a celebrated Fourier whose name is forgotten now, and in some attic an obscure Fourier who will be remembered in times to come.

The first is Joseph Fourier and the second is the utopist Charles Fourier. Clearly Victor Hugo did not consider Joseph Fourier as a “gloire nationale”. He was a friend of François Arago, who succeeded Fourier as “secrétaire perpétuel de l’Académie des sciences”. After the death of Fourier in 1830, Arago wrote an obituary in this quality, and Victor Cousin as member of the Académie Française. Both obituaries are very rich and interesting about the life of Joseph Fourier, but both ignore or underestimate his work as a mathematician. Arago, who was elected very young and long before Fourier as a member of the Academy of sciences, likely remembered that Lagrange was very reluctant towards the decomposition of a function into a trigonometric series and knew that the Prize given to Fourier in 1811 for the Analytical Theory of Heat expressed reservations on this theory, both from the point of view of generality and of rigor. Fourier had competitors like Cauchy and Poisson. All that can explain why the obituary by Arago looked as a beautiful burial.

Actually, the French did not recognize the importance of Joseph Fourier until recently. There is a “rue Charles Fourier” in Paris, no street Joseph Fourier. In the first editions of Encyclopaedia Universalis, the French equivalent to Encyclopaedia Britannica, there was no article on Joseph Fourier; it was still the case in the sixth edition in 1974. I already said that Darboux published only a part of his work in mathematics, essentially the Analytical Theory of Heat, and the Collected Works were never published. Until recently, the life and works of Joseph Fourier did not attract much attention in France, at least outside Grenoble; in Grenoble, the Institute of Mathematics was called Institut Fourier a long time ago, and the whole university to which it belongs was called Université Joseph Fourier in 1987. In 1998, an excellent book appeared: “Fourier, créateur de la physique mathématique”, by a mathematician, Jean Dhombres, and a physicist, Jean-Bernard Robert. There are signs that the name of Joseph Fourier is not forgotten anymore in France.

2.2 Jacobi

More important is the appreciation of Carl Gustav Jacobi, then 26, a few weeks after the death of Fourier. In a letter to Legendre he wrote:

> M. Poisson n’aurait pas dû reproduire dans son rapport une phrase peu adroite de feu M. Fourier, où ce dernier nous reproche, à Abel et à moi, de ne pas nous être occupés de préférence du mouvement de la chaleur. Il est vrai que M. Fourier avait l’opinion que le but principal des mathématiques était l’utilité publique et l’explication des phénomènes naturels; mais un philosophe comme lui aurait dû saisir que le but unique de la science, c’est l’honneur de l’esprit humain, et que, sous ce titre, une question de nombres vaut autant qu’une question de système du monde.
>
> (Jacobi, lettre à Legendre, 2 juillet 1830)

> M. Poisson should not have reproduced an ill-timed appreciation of the late M. Fourier, reproaching Abel and me for not paying enough attention to the movement of heat. In truth, M. Fourier thought that public interest and explanation of natural phenomena were the main purpose of mathematics. But, as a philosopher, he should have known that the unique purpose of science is the honour of the human mind, and that, in this respect, a question about numbers is as valuable as a question about the universe.

The key word "l'honneur de l'esprit humain" became a motto for pure mathematics, in opposition with Fourier's point of view. In particular, it gave the title of a famous book of Jean Dieudonné.

2.3 Fourier

The point of view of Fourier is expressed very clearly in a few sentences of the general introduction ("Discours préliminaire") of his Analytical Theory of Heat. Here is a selection of such sentences:

> Les équations du mouvement de la chaleur, comme celles qui expriment les vibrations des corps sonores, ou les dernières oscillations ds liquides, appartiennent à une des branches de la science du calcul les plus récemment découvertes... Après avoir établi ces équations différentielles, il fallait en obtenir les intégrales; ce qui consiste à passer d'une expression commune à une solution propre assujettie à toutes les conditions données. Cette recherche difficile exigeait une analyse spéciale, fondée sur des théorèmes nouveaux... La méthode qui en dérive ne laisse rien de vague ni d'indéterminé dans les solutions. Elle les conduit jusqu'aux dernières applications numériques, condition nécessaire de toute recherche, et sans lesquelles on n'arriverait qu'à des transformations inutiles...
>
> (Joseph Fourier [2], Discours préliminaire)

> L'étude approfondie de la nature est la source la plus féconde des découvertes mathématiques...
>
> Les équations analytiques... s'étendent à tous les phénomènes généraux. Il ne peut y avoir de langage plus universel et plus simple, plus exempt d'erreurs et d'obscurités, c'est-à-dire plus digne d'exprimer les rapports invariables des êtres naturels.
>
> Considérée de ce point de vue, l'analyse mathématique est aussi étendue que la nature elle même... Son attribut principal est la clarté. Elle n'a point de signes pour exprimer les notions confuses. Elle rapproche les phénomènes les plus divers et découvre les analogies secrètes qui unissent... Elle nous les rend présents et mesurables, et semble être une faculté de la raison humaine, destinée à suppléer à la brièveté de la vie et à l'imperfection des sens. (ibid)

Let me begin with the second excerpt:

> The thorough study of nature is the most productive source of mathematical discoveries.
>
> Analytic equations apply to all general phenomena. There is no simpler and more universal language, more free from errors, and more able to express permanent relations between natural bodies.
>
> From this point of view mathematical analysis is as large as nature itself. Its main feature is clarity. It has no sign for confuse notions. It connects the most diverse phenomena and expresses their hidden analogies. It makes them accessible and measurable, and it seems to be a faculty of the human brain, making up for the brevity of life and imperfection of our senses.

This is a glorious definition of mathematical analysis. By the way, Fourier was interested also by the human life and industry, and this, parallel to "the thorough study of nature", was another important source of his mathematical investigations and discoveries.

Here is an approximative translation of the first excerpt:

> The heat equation, as well as the equations concerning vibrating strings or motions of liquids, belongs to a quite recent brand of analysis [namely, PDE]. After establishing the equations one has to find the solutions, that is, go from a general expression to a particular solution subject to prescribed conditions. This investigation was difficult and needed a new kind of analysis, based on new theorems... The corresponding method leaves nothing vague in the solutions. It leads to final numerical applications, as any investigation should do in order to be useful.

The Fourier approach is very well described in the Discours préliminaire: start from natural phenomena and end with numerical conclusions. In between "a new kind of analysis" is needed, what we call now Fourier analysis. This sounds more modern now, with modeling and computers, than 50 years ago, and explains the comeback of Fourier's views.

2.4 Dirichlet and Riemann

The main continuators of Fourier were Dirichlet and Riemann. Dirichlet met Fourier when he stayed in Paris, between 1822 and 1825, not yet 20 years old. In 1829, he published the first general and correct statement about the convergence of Fourier series. The beginning of this article was a tribute payed to Fourier ("l'illustre géomètre qui a ouvert une nouvelle carrière aux applications de l'analyse") and a criticism of the approach of the convergence problem by Cauchy. For Dirichlet as for Fourier, the starting point was a function given in some way. Then came integral formulas providing the coefficients of a trigonometric series. The problem was to show that this trigonometric series converges to the function.

The treatment of the problem by Dirichlet was a masterpiece of analysis, and it led to the celebrated Dirichlet conditions. It led also to an important remark: the given function needs to satisfy some conditions in order that the integral formulas make sense. As a comment, Dirichlet introduced his famous example of a function taking a value on rational points and another on irrational points: for him as later for Riemann, such a function is not integrable on any interval.

Since Dirichlet the *convergence problem* of Fourier series (that is, trigonometric series whose coefficients are given by the Fourier integral formulas) is linked to two major questions: what do you mean by a *function*? What do you mean by an *integral*?

Actually, the term *Fourier series* ("Fouriersche Reihe") appears for the first time in the dissertation of Riemann on trigonometric series, written in 1854. The beginning of the dissertation is a history of the subject from the controversy on vibrating strings in the 18^{th} century to the article by Dirichlet, with comments and remarks, on analytic and harmonic continuation on one hand, and ordinary and absolute convergence of numerical series on the other, inspired by the mistakes of Cauchy. A few pages are devoted to ordinary and generalized integrals. The Riemann integral of a bounded function on a bounded interval is defined in a few lines, and (before Lebesgue!) Riemann gives an explicit necessary and sufficient condition for a function to be integrable.

A leitmotiv of Riemann's dissertation is the recognition of the role of Fourier. After the controversy on vibrating strings in which d'Alembert, Euler, Daniel Bernoulli and Lagrange took part, "for almost 50 years the question of representing an arbitrary function by an analytic expression did not make any essential progress. Then a remark of Fourier gave this question a new look, and a new epoch began in this part of mathematics, which proved soon of exceptional importance in the development of mathematical physics. Fourier remarked that, given a trigonometric series $f(x) = \dots$, the coefficients are well-defined by the formulas $a_n = \dots$, $b_n = \dots$. He observed that this definition of the series makes sense for quite arbitrary functions $f(x)$; taking for $f(x)$ a so-called discontinuous function (the ordinate of a broken line above the abscissa x), he obtained a series that actually gave always the value of the function."

Then, after discussing why Lagrange was reluctant and Poisson hostile, Riemann states that "it was Fourier who actually recognized the nature of trigonometric series in a complete and correct way; since then they were applied many times in mathematical physics for representing arbitrary functions, and one can be easily convinced in each particular case that the Fourier series converges indeed to the value of the function."

A general proof was needed. After the attempt by Cauchy, this was realized by Dirichlet for a large class of functions, covering (Riemann said) all possible needs of physics. Nevertheless "the application of Fourier series is not restricted to researches in physics; they are now applied successfully in a domain of pure mathematics, the theory of numbers, where it seems that the most important functions are not those considered by Dirichlet." Here are the exact quotations of Riemann.

> Fast fünfzig Jahre vergingen, ohne dass in der Frage über die analytische Darstellbarkeit willkürlicher Functionen ein wesenticher Fortschritt gemacht wurde. Da warf eine Bemerkung Fourier's ein neues Licht auf diesen Gegenstand; eine neue Epoche in der Entwicklung dieses Teils der Mathematik begann, die sich bald auch äusserlich in grossartigen Erweiterungen der mathematischen Physik kund tat. Fourier bemerkte, dass in der trigonometrischen Reihe
>
> $$f(x) = a_1 \sin x + a_2 \sin 2x + \cdots + \tfrac{1}{2} b_0 + b_1 \cos x + b_2 \cos 2x + \cdots \ ,$$
>
> die Coefficienten sich durch die Formeln
>
> $$a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin nx \, \mathrm{d}x \ , \qquad b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos nx \, \mathrm{d}x \ ,$$
>
> bestimmten lassen. Er sah, dass diese Bestimmungsweise auch anwendbar bleibe, wenn die Function $f(x)$ ganz willkürlich sei; er setzte für $f(x)$ eine so genannte discontinuirliche Function (die Ordinate einer gebrochenen Linie für die Abcissa x) and erhielt eine Reihe, welche in der That stets den Wert der Function gab.
>
> (Bernhard Riemann [9])

> Durch Fourier was nun zwar die Natur der trigonometrischen Reihen vollkommen richtig erkannt; sie wurden seitdem in der mathematischen Physik zur Darstellung willkürlicher Functionen vielfach angewandt, und in jedem einzelnen Falle überzeugte man sich leicht, dass die Fouriersche Reihe wirklich gegen den Werth der Function convergire. (ibid)

> Zweitens aber ist die Anwendbarkeit der Fourierschen Reihen nicht auf physikalische Untersuchungen beschränkt; sie ist jetzt auch in einem Gebiete der seinen Mathematik, der Zahlentheorie, mit Erfolg angewandt, and hier scheinen gerade diejenigen Funktionen, deren Darstellbarkeit durch eine trigonometrische Reihe Dirichlet nicht untersucht hat, von Wichtigkeit zu sein. (ibid)

3 The Riemann Theory of Trigonometric Series

However, the main and most original part of Riemann's dissertation does not follow the lines traced by Fourier and Dirichlet. Instead of starting from a function and looking for the properties of the Fourier series, in particular the convergence problem, Riemann started from an everywhere convergent trigonometric series and looked for the properties of the sum as a function. The machinery that he created is known as the Riemann theory of trigonometric series. It implies double formal integration of the given series and formal multiplication by sufficiently regular series (or functions): viewed from now, it is an anticipation of the treatment of Schwartzs distributions. More directly, it anticipates the "smooth functions" of Zygmund and the "pseudomeasures" and "pseudofunctions" of Kahane and Salem.

The Riemann theory of trigonometric series played a major role in the history of mathematics because of two questions that Riemann left open and that were solved by Georg Cantor: prove that, if an everywhere convergent trigonometric series converges everywhere, its coefficients tend to zero, and, more difficult, that if it converges everywhere to zero it is the null series. This last statement is the "uniqueness theorem" of Cantor. Then Cantor looked for an "extension": is the result valid when the assumption is weakened in the form that the series converges to zero out of a given set? Cantor proved that it was the case for "reducible" sets (with countable closure). It was his first opportunity to develop his theory of real numbers and real sets, so that trigonometric series appear as the first historical source of the theory of sets.

Sets of uniqueness (for which the answer to the question is positive) and sets of multiplicity (the opposite) became a favorite field for applying methods coming from real and functional analysis, probability, number theory, and logics. The main contributors were Lebesgue, Marcel Riesz, Young, Menchoff, Rajchman, Bari, Zygmund, Marcinkiewicz, Salem, then R. Kaufman, T. Körner, J.-P. Kahane, B. Mandelbrot, Y. Katznelson, B. Connes, and more recently A.S. Kechris and A. Louveau, G. Debs and J. Saint-Raymond, J. Bourgain, M. Ash and G. Wang. A brief history of the subject can be found in [4].

The uniqueness theorem of Cantor means that, given the sum of an everywhere convergent trigonometric series, the coefficients are well-defined. In order to compute them, a new kind of Fourier formulas is needed, with a new meaning for the integral. It is the purpose of the second "totalization" theory of A. Denjoy, and his "Leçons sur le calcul des coefficients d'une série trigonométriques" (1941, 1949) is a complete exposition of the subject, in four books.

4 The Convergence Problem After Dirichlet

The Riemann theory and the Cantor uniqueness theorem are part of the heritage of Fourier, but not in the main direction.

The main direction was well described by Riemann himself. It is the direction explored by Dirichlet, the convergence problem.

Dirichlet believed that the Fourier series of a continuous function should converge pointwise to the function, though he was not able to prove it. This was disproved only in 1873, by Paul du Bois-Raymond. He constructed a continuous function whose Fourier series diverges at a given point. The construction is a kind of "condensation of singularities". Variations were given by Lebesgue and by Fejer. Today it appears as a standard application of the Banach–Steinhaus theorem, using the fact that the L^1–norms of the Dirichlet kernel (the so-called "Lebesgue constants") are not bounded.

Is it possible to construct a continuous function whose Fourier series diverges everywhere? The question was still open in 1965, before the Carleson theorem, and Katznelson and I proved that either it is the case, or the Fourier series of any continuous function converges almost everywhere to the function. The key was to construct a continuous function whose Fourier series diverges on a given null-set.

4.1 The Carleson Theorem

The question was settled by the Carleson theorem of 1966: the Fourier series of a continuous function converges to the function almost everywhere and nothing better can be said for continuous functions [1]. But much more can be said, by enlarging the class of functions. Carleson proved that the result holds for L^2 (1966), and R. Hunt for L^p with $p > 1$ (1967). On the other hand, the result does not hold for L^1, since Kolmogorov constructed an L^1–function whose Fourier series diverges almost everywhere (1922) and even everywhere (1926). The situation near L^1 was investigated recently and raises some puzzling questions, as we shall see later.

In order to understand the importance of Carleson–Hunt in 1966–67, let us consult the successive editions and impressions of Zygmund's book "Trigonometric series" [11]. For general L^2–functions, the best known result before 1966 was due to Kolmogorov (1922): given a Hadamard lacunary sequence (n_k), for example $n_k = 2^k$, the partial sums of order n_k tend to the function almost everywhere. For general L^p–functions, $p > 1$, the same holds but the proof relies on a highly sophisticated machinery, the Littlewood–Paley theory (1938). Two chapters of the second edition of Zygmund's book are devoted to the Littlewood–Paley theory and to what was considered as its main application, the almost everywhere convergence of partial sums of order n_k. The discovery of Carleson changed the landscape in a drastic way. First, Kolmogorov's result was not the best anymore. Second, due to Hunt's extension of Carleson's theorem for all L^p, $p > 1$, the Littlewood–Paley theorem became obsolete as a means to study the convergence problem. This was a shock for Zygmund. There were several new "impressions" of the second edition of "Trigonometric series" during his life-time, but no "third edition". A "third edition" would have been a complete rewriting of the book: Carleson–Hunt would have been included, and many partials results and related methods dropped; there would have been no reason to keep the Littlewood–Paley theory. Fortunately, Zygmund gave up such a rewriting and the book was kept with its beautiful exposition of the Littlewood–Paley theory, without Carleson–Hunt.

The situation near L^1 is in close relation with the asymptotic behaviour of the partial sums $S_n(f,x)$ when f belongs to L^1. The first important result is due to Hardy (1913): if $f \in L^1$, $S_n(f,x) = o(\log n)$ almost everywhere. Hardy conjectured that it was a best possible result. In the opposite direction, the Kolmogorov example of 1926 establishes the existence of $f \in L^1$ such that $\lim |S_n(f,x)| = \infty$ everywhere. For which increasing sequences $\ell(n)$ is it true that there exists $f \in L^1$ such that $\lim(|S_n(f,x)|/\ell(n)) = \infty$ everywhere? Until a few years ago, the best result was that $\ell(n) = o(\log\log n)$ works (Chen 1962). In 1999, Konyagin [8] went as far as $\ell(n) = o((\log n/\log\log n)^{1/2})$, and Bochkarev proved in 2003 that $\ell(n) = o((\log n)^{1/2})$ is sufficient when the circle is replaced by the Cantor group. It is a challenging problem now to improve either Hardy or Konyagin. A test case is $\ell(n) = (\log n)^p$ with $1/2 < p < 1$.

4.2 Variations About Convergence

The revival of Fourier series in the twentieth century is due in a large part to other ways to consider the convergence problem.

In the first place one can introduce summability processes instead of ordinary convergence. This way was opened by Fejer in 1900 and it led to positive kernels, approximate identities, multipliers and convolution. The most important notion, convolution, was formalized rather late and actually no formal definition covers the real range of the notion. It became better understood with the convolution algebras of Wiener, one of the sources of the normed rings (Banach algebras) of Gelfand.

On the other hand convergence can be considered in spaces of functions, and summability as well. This direction created a strong link between Fourier series and the beginning of functional analysis. The initial impulse was the Lebesgue integral (1901) and its application to Fourier series (1906), followed by the Riesz–Fischer theorem (1907). The simple statement "L^p is complete" (needing first the definitions of L^p–spaces and complete metric spaces) belongs to the heritage of Fourier.

Fourier series are a prototype of orthogonal series, and orthogonal series appear in all parts of analysis. The L^2–convergence is guaranteed, but problems on almost everywhere convergence are quite interesting, parallel to those on classical Fourier series.

Thousands of papers and hundreds of books being written on these subjects, I shall not insist on them any more.

5 Fourier Comes Back

Let us go back to Fourier.

His first and typical use of trigonometric series was a solution of a problem on the distribution of temperatures in a given solid body, a cylinder based on the half strip $-\pi/2 \le x \le \pi/2$, $0 \le y < \infty$, with $-\infty < z < \infty$. The horizontal basis ($y = 0$) is at temperature 1, the vertical edges ($x = \pm\pi/2$) at temperature 0. At the state of equilibrium the temperature $u(x, y)$ satisfies

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \; ,$$

with $u(\pm\pi/2, y) = 0$ and $u(x, 0) = 1$ $(-\pi/2 < x < \pi/2)$. A formal solution is

$$u(x, y) = a_1 \mathrm{e}^{-y} \cos x + a_3 \mathrm{e}^{-3y} \cos 3x + a_5 \mathrm{e}^{-5y} \cos 5x + \cdots \tag{1}$$

and the last requirement is expressed by the condition

$$1 = a_1 \cos x + a_3 \cos 3x + a_5 \cos 5x + \cdots \qquad (-\pi/2 < x < \pi/2) \; . \tag{2}$$

Before writing the integral formulas for the coefficients, Fourier computed them in a strange way: differentiation, truncation, solution of a linear system. Darboux said that this was a natural method and he was right. What Fourier did was to look at trigonometric polynomials $1 - \sum a_n \cos nx$ (n odd) of a given degree that are as flat as possible at 0, and compute the limits of the a_n when the degree increases to infinity, namely $(-1)^{n+1} 4/\pi n$. The derivatives of these trigonometric polynomials are as flat as possible at 0, odd, and their integral on $(-\pi/2, 0)$ is 1. In the sense of distributions they converge to $2(\delta_{-\pi/2} - \delta_{\pi/2})$, and this is enough in order to establish (1) when $y > 0$. The proof of (2) is more delicate.

Of course, Fourier did not know the theory of distributions. But he had a flair for the meaning of computations, and it may be wise to try to understand what he did before condemning his methods and statements.

After giving the integral formulas Fourier observes that, due to the exponential factors, the series (1) is very rapidly convergent when $y > 0$ ("très convergente", "extrèment convergente"). About series (2) he says that convergence can be proved ("on démontre rigoureusement") and actually he gives a correct proof later in the chapter.

Then he extends the procedure to other functions, gives the Fourier formulas for general 2π–periodic functions, and states that this applies to arbitrary functions and gives trigonometric series which always converge to the functions. In a formal way this is wrong, and we just discussed some of the main contributions of mathematicians in order to find the correct notions and statements. Fourier was criticized, by Darboux in particular, for being inaccurate in some of his statements, and that explains in part why he was so long in disfavour with French people. But Fourier deserves to be appreciated not because he proved theorems and made perfect statements, but in the way he launched a long-term program in mathematics.

Examples can be found in all parts of The Analytical Theory of Heat, of statements that were considered as absurd and may also sound prophetic. Here is one ([2] Chap. III, pp. 235). From the integral formulas for coefficients Fourier derives the formula

$$F(x) = \frac{1}{\pi} \int_{-\pi}^{\pi} F(\alpha) \mathrm{d}\alpha \left(\frac{1}{2} + \sum_i \cos i(x-\alpha) \right) .$$

The comment of Darboux is that the parenthesis has no possible meaning. However, here is Fourier's explanation:

> L'expression (...) représente une fonction de x et de α telle que, si on la multiplie par une fonction quelconque $F(\alpha)$ et si, après avoir écrit dα, on intégre entre les limites $\alpha = -\pi$ et $\alpha = \pi$, on aura changé la fonction proposée $F(\alpha)$ en une pareille fonction de x, multipliée par la demi-circonférence. On verra par la suite quelle est la nature de ces quantités, telles que $1/2 + \sum \cos i(x-\alpha)$, qui jouissent de la propriété que l'on vient d'énoncer.

Clearly, I believe, Fourier had the intuition of the Dirac measure and the way to use it (in particular, in later sections, derivation and representation as a Fourier integral).

It should be noted that the first exposition by Laurent Schwartz of his theory of distributions is an article (1946) entitled "Généralisation de la notion de fonction, de dérivation, de transformation de Fourier, et applications mathématiques et physiques" [10]. In a way, the theory of distributions belongs to the heritage of Fourier.

I shall be brief on more recent and spectacular reincarnations of Fourier series. The Fast Fourier Transform of Cooley and Tuckey (1965), presented as "An algorithm for the machine calculation of complex Fourier series", has invaluable applications in all parts of science, from astrophysics to biology.

The wavelets of Yves Meyer (1985) came from physicists and engineers, and soon created a common ground for specialists of different fields of science and industry. The story is well known and still in progress[1] and there is no point in telling it again.

As far as the heritage of Fourier is concerned, the main point is that FFT and wavelets testify that the philosophy of Fourier, expressed in the excerpts of the Discours préliminaire I gave above, makes a spectacular come-back.

I indicated at the beginning that I would restrict the heritage of Fourier to his work as a mathematician and, to be more specific, to Fourier series. I chose, actually, a very few points of interest in the history of Fourier series, and I hardly mentioned *one* open problem. My oral communication was not organized exactly in that way. But I feel better now to contribute to "Perspectives in Analysis" by a reflection on the past than by a list of open problems according to my taste. The past is very rich and the way in which it echoes the most recent research in mathematics is actually part of "Perspectives in Analysis".

[1] See Jaffard et al. [3] for example.

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The Quantum-Mechanical Many-Body Problem: The Bose Gas

Elliott H. Lieb[1], Robert Seiringer[2], Jan Philip Solovej[3], and Jakob Yngvason[4]

[1] Departments of Mathematics and Physics, Princeton University, Jadwin Hall, P.O. Box 708, Princeton, NJ 08544, USA. lieb@math.princeton.edu
[2] Department of Physics, Princeton University, Jadwin Hall, P.O. Box 708, Princeton, NJ 08544, USA. rseiring@math.princeton.edu
[3] School of Mathematics, Institute for Advanced Study, 1 Einstein Dr., Princeton, N.J. 08540. On leave from Dept. of Math., University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen, Denmark. solovej@math.ku.dk
[4] Institut für Theoretische Physik, Universität Wien, Boltzmanngasse 5, A-1090 Vienna, Austria. yngvason@thor.thp.univie.ac.at

Summary. Now that the low temperature properties of quantum-mechanical many-body systems (bosons) at low density, ρ, can be examined experimentally it is appropriate to revisit some of the formulas deduced by many authors 4–5 decades ago, and to explore new regimes not treated before. For systems with repulsive (i.e. positive) interaction potentials the experimental low temperature state and the ground state are effectively synonymous – and this fact is used in all modeling. In such cases, the leading term in the energy/particle is $2\pi\hbar^2 a\rho/m$ where a is the scattering length of the two-body potential. Owing to the delicate and peculiar nature of bosonic correlations (such as the strange $N^{7/5}$ law for charged bosons), four decades of research failed to establish this plausible formula rigorously. The only previous lower bound for the energy was found by Dyson in 1957, but it was 14 times too small. The correct asymptotic formula has been obtained by us and this work will be presented. The reason behind the mathematical difficulties will be emphasized. A different formula, postulated as late as 1971 by Schick, holds in two dimensions and this, too, will be shown to be correct. With the aid of the methodology developed to prove the lower bound for the homogeneous gas, several other problems have been successfully addressed. One is the proof by us that the Gross-Pitaevskii equation correctly describes the ground state in the 'traps' actually used in the experiments. For this system it is also possible to prove complete Bose condensation and su-

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perfluidity, as we have shown. On the frontier of experimental developments is the possibility that a dilute gas in an elongated trap will behave like a one-dimensional system; we have proved this mathematically. Another topic is a proof that Foldy's 1961 theory of a high density Bose gas of charged particles correctly describes its ground state energy; using this we can also prove the $N^{7/5}$ formula for the ground state energy of the two-component charged Bose gas proposed by Dyson in 1967. All of this is quite recent work and it is hoped that the mathematical methodology might be useful, ultimately, to solve more complex problems connected with these interesting systems.

Foreword

At the conference "Perspectives in Analysis" at the KTH, Stockholm, June 23, 2003, one of us (E.H.L.) contributed a talk with the title above. This talk covered material by all the authors listed above. This contribution is a much expanded version of the talk and of [47]. It is based on, but supersedes, the article [52].[1]

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[1] Note added in proof: A more extensive version of these notes, together with developments obtained after submission of the manuscript, recently appeared in the book: E.H. Lieb, R. Seiringer, J.P. Solovej and J. Yngvason, *The Mathematics of the Bose Gas and its Condensation*, vol. **34**, Oberwolfach Seminars Series, Birkhäuser (2005).

1 Introduction

Schrödinger's equation of 1926 defined a new mechanics whose Hamiltonian is based on classical mechanics, but whose consequences are sometimes non-intuitive from the classical point of view. One of the most extreme cases is the behavior of the ground (= lowest energy) state of a many-body system of particles. Since the ground state function $\Psi(\mathbf{x}_1, ..., \mathbf{x}_N)$ is automatically symmetric in the coordinates $\mathbf{x}_j \in \mathbb{R}^3$ of the N particles, we are dealing necessarily with *'bosons'*. If we imposed the Pauli exclusion principle (anti-symmetry) instead, appropriate for electrons, the outcome would look much more natural and, oddly, more classical. Indeed, the Pauli principle is *essential* for understanding the stability of the ordinary matter that surrounds us.

Recent experiments have confirmed some of the bizarre properties of bosons close to their ground state, but the theoretical ideas go back to the 1940's – 1960's. The first sophisticated analysis of a gas or liquid of *interacting* bosons is due to Bogolubov in 1947. His approximate theory as amplified by others, is supposed to be exact in certain limiting cases, and some of those cases have now been verified rigorously (for the ground state energy) — 3 or 4 decades after they were proposed.

The discussion will center around five main topics.

1. The dilute, homogeneous Bose gas with repulsive interaction (2D and 3D).
2. Repulsive bosons in a trap (as used in recent experiments) and the "Gross–Pitaevskii" equation.
3. Bose condensation and superfluidity for dilute trapped gases.
4. One-dimensional behavior of three-dimensional gases in elongated traps.
5. Foldy's "jellium" model of charged particles in a neutralizing background and the extension to the two-component gas.

Note that for potentials that tend to zero at infinity 'repulsive' and 'positive' are synonymous — in the quantum mechanical literature at least. In classical mechanics, in contrast, a potential that is positive but not monotonically decreasing is not called repulsive.

The discussion below of topic 1 is based on [62] and [63], and of topic 2 on [53] and [54]. See also [64, 55, 78, 56].

The original references for topic 3 are [51] and [57], but for transparency we also include here a section on the special case when the trap is a rectangular box. This case already contains the salient points, but avoids several complications due the inhomogeneity of the gas in a general trap. An essential technical tool for topic 3 is a generalized Poincaré inequality, which is discussed in a separate section.

Topic 4 is a summary of the work in [58].

The discussion of topic 5 is based on [60] and [61].

Topic 1 (3-dimensions) was the starting point and contains essential ideas. It is explained here in some detail and is taken, with minor modifications (and corrections), from [64]. In terms of technical complexity, however, the fifth topic is the most involved and can not be treated here in full detail.

The interaction potential between pairs of particles in the Jellium model in topic 5 is the repulsive, *long-range* Coulomb potential, while in topics 1–4 it is assumed to be repulsive and *short range*. For alkali atoms in the recent experiments on Bose Einstein condensation the interaction potential has a repulsive hard core, but also a quite deep attractive contribution of van der Waals type and there are many two body bound states [69]. The Bose condensate seen in the experiments is thus not the true ground state (which would be a solid) but a metastable state. Nevertheless, it is usual to model this metastable state as the ground state of a system with a repulsive two body potential having the same scattering length as the true potential, and this is what we shall do. In this paper all interaction potentials will be positive.

2 The Dilute Bose Gas in 3D

We consider the Hamiltonian for N bosons of mass m enclosed in a cubic box Λ of side length L and interacting by a spherically symmetric pair potential $v(|\mathbf{x}_i - \mathbf{x}_j|)$:

$$H_N = -\mu \sum_{i=1}^{N} \Delta_i + \sum_{1 \le i < j \le N} v(|\mathbf{x}_i - \mathbf{x}_j|) \ . \tag{2.1}$$

Here $\mathbf{x}_i \in \mathbb{R}^3$, $i = 1, \ldots, N$ are the positions of the particles, Δ_i the Laplacian with respect to $\mathbf{x}_i$, and we have denoted $\hbar^2/2m$ by μ for short. (By choosing suitable units μ could, of course, be eliminated, but we want to keep track of the dependence of the energy on Planck's constant and the mass.) The Hamiltonian (2.1) operates on *symmetric* wave functions in $L^2(\Lambda^N, \mathrm{d}\mathbf{x}_1 \cdots \mathrm{d}\mathbf{x}_N)$ as is appropriate for bosons. The interaction potential will be assumed to be *nonnegative* and to decrease faster than $1/r^3$ at infinity.

We are interested in the ground state energy $E_0(N, L)$ of (2.1) in the *thermodynamic limit* when N and L tend to infinity with the density $\rho = N/L^3$ fixed. The energy per particle in this limit is

$$e_0(\rho) = \lim_{L \to \infty} E_0(\rho L^3, L)/(\rho L^3) \ . \tag{2.2}$$

Our results about $e_0(\rho)$ are based on estimates on $E_0(N, L)$ for finite N and L, which are important, e.g., for the considerations of inhomogeneous systems in [53]. To define $E_0(N, L)$ precisely one must specify the boundary conditions. These should not matter for the thermodynamic limit. To be on the safe side we use Neumann boundary conditions for the lower bound, and Dirichlet boundary conditions for the upper bound since these lead, respectively, to the lowest and the highest energies.

For experiments with dilute gases the *low density asymptotics* of $e_0(\rho)$ is of importance. Low density means here that the mean interparticle distance,

$\rho^{-1/3}$ is much larger than the *scattering length* a of the potential, which is defined as follows. The zero energy scattering Schrödinger equation

$$-2\mu\Delta\psi + v(r)\psi = 0 \tag{2.3}$$

has a solution of the form, asymptotically as $|\mathbf{x}| = r \to \infty$ (or for all $r > R_0$ if $v(r) = 0$ for $r > R_0$),

$$\psi_0(\mathbf{x}) = 1 - a/|\mathbf{x}| \tag{2.4}$$

(The factor 2 in (2.3) comes from the reduced mass of the two particle problem.) Writing $\psi_0(\mathbf{x}) = u_0(|\mathbf{x}|)/|\mathbf{x}|$ this is the same as

$$a = \lim_{r\to\infty} r - \frac{u_0(r)}{u_0'(r)}\,, \tag{2.5}$$

where u_0 solves the zero energy (radial) scattering equation,

$$-2\mu u_0''(r) + v(r)u_0(r) = 0 \tag{2.6}$$

with $u_0(0) = 0$.

An important special case is the hard core potential $v(r) = \infty$ if $r < a$ and $v(r) = 0$ otherwise. Then the scattering length a and the radius a are the same.

Our main result is a rigorous proof of the formula

$$e_0(\rho) \approx 4\pi\mu\rho a \tag{2.7}$$

for $\rho a^3 \ll 1$, more precisely of

Theorem 2.1 (Low density limit of the ground state energy).

$$\lim_{\rho a^3\to 0} \frac{e_0(\rho)}{4\pi\mu\rho a} = 1\,. \tag{2.8}$$

This formula is independent of the boundary conditions used for the definition of $e_0(\rho)$. It holds for every positive radially symmetric pair potential such that $\int_R^\infty v(r)r^2\mathrm{d}r < \infty$ for some R, which guarantees a finite scattering length, cf. Appendix A in [63].

The genesis of an understanding of $e_0(\rho)$ was the pioneering work [7] of Bogolubov, and in the 50's and early 60's several derivations of (2.8) were presented [36], [44], even including higher order terms:

$$\frac{e_0(\rho)}{4\pi\mu\rho a} = 1 + \tfrac{128}{15\sqrt{\pi}}(\rho a^3)^{1/2} + 8\left(\tfrac{4\pi}{3} - \sqrt{3}\right)(\rho a^3)\log(\rho a^3) + O(\rho a^3) \tag{2.9}$$

These early developments are reviewed in [45]. They all rely on some special assumptions about the ground state that have never been proved, or on the selection of special terms from a perturbation series which likely diverges. The only rigorous estimates of this period were established by Dyson, who derived the following bounds in 1957 for a gas of hard spheres [17]:

$$\frac{1}{10\sqrt{2}} \leq \frac{e_0(\rho)}{4\pi\mu\rho a} \leq \frac{1+2Y^{1/3}}{(1-Y^{1/3})^2} \tag{2.10}$$

with $Y = 4\pi\rho a^3/3$. While the upper bound has the asymptotically correct form, the lower bound is off the mark by a factor of about 1/14. But for about 40 years this was the best lower bound available!

Under the assumption that (2.8) is a correct asymptotic formula for the energy, we see at once that understanding it physically, much less proving it, is not a simple matter. Initially, the problem presents us with two lengths, $a \ll \rho^{-1/3}$ at low density. However, (2.8) presents us with another length generated by the solution to the problem. This length is the de Broglie wavelength, or 'uncertainty principle' length (sometimes called 'healing length')

$$\ell_c \sim (\rho a)^{-1/2} \ . \tag{2.11}$$

The reason for saying that ℓ_c is the de Broglie wavelength is that in the hard core case all the energy is kinetic (the hard core just imposes a $\psi = 0$ boundary condition whenever the distance between two particles is less than a). By the uncertainty principle, the kinetic energy is proportional to an inverse length squared, namely ℓ_c. We then have the relation (since ρa^3 is small)

$$a \ll \rho^{-1/3} \ll \ell_c \tag{2.12}$$

which implies, physically, that it is impossible to localize the particles relative to each other (even though ρ is small). Bosons in their ground state are therefore 'smeared out' over distances large compared to the mean particle distance and their individuality is entirely lost. They cannot be localized with respect to each other without changing the kinetic energy enormously.

Fermions, on the other hand, prefer to sit in 'private rooms', i.e., ℓ_c is never bigger than $\rho^{-1/3}$ by a fixed factor. In this respect the quantum nature of bosons is much more pronounced than for fermions.

Since (2.8) is a basic result about the Bose gas it is clearly important to derive it rigorously and in reasonable generality, in particular for more general cases than hard spheres. The question immediately arises for which interaction potentials one may expect it to be true. A notable fact is that it *is not true for all* v with $a > 0$, since there are two body potentials with positive scattering length that allow many body bound states. (There are even such potentials without two body bound states but with three body bound states [3].) For such potentials (2.8) is clearly false. Our proof, presented in the sequel, works for nonnegative v, but we conjecture that (2.8) holds if $a > 0$ and v has no N-body bound states for any N. The lower bound is, of course, the hardest part, but the upper bound is not altogether trivial either.

Before we start with the estimates a simple computation and some heuristics may be helpful to make (2.8) plausible and motivate the formal proofs.

With ψ_0 the zero energy scattering solution, partial integration, using (2.3) and (2.4), gives, for $R \geq R_0$,

$$\int_{|\mathbf{x}|\leq R} \{2\mu|\nabla\psi_0|^2 + v|\psi_0|^2\}\mathrm{d}\mathbf{x} = 8\pi\mu a \left(1 - \frac{a}{R}\right) \to 8\pi\mu a \quad \text{for } R \to \infty \,. \tag{2.13}$$

Moreover, for positive interaction potentials the scattering solution minimizes the quadratic form in (2.13) for each $R \geq R_0$ with the boundary condition $\psi_0(|\mathbf{x}| = R) = (1 - a/R)$. Hence the energy $E_0(2, L)$ of two particles in a large box, i.e., $L \gg a$, is approximately $8\pi\mu a/L^3$. If the gas is sufficiently dilute it is not unreasonable to expect that the energy is essentially a sum of all such two particle contributions. Since there are $N(N-1)/2$ pairs, we are thus lead to $E_0(N, L) \approx 4\pi\mu a N(N-1)/L^3$, which gives (2.8) in the thermodynamic limit.

This simple heuristics is far from a rigorous proof, however, especially for the lower bound. In fact, it is rather remarkable that the same asymptotic formula holds both for ‘soft’ interaction potentials, where perturbation theory can be expected to be a good approximation, and potentials like hard spheres where this is not so. In the former case the ground state is approximately the constant function and the energy is *mostly potential*: According to perturbation theory $E_0(N, L) \approx N(N-1)/(2L^3) \int v(|\mathbf{x}|)\mathrm{d}\mathbf{x}$. In particular it is *independent of* μ, i.e. of Planck's constant and mass. Since, however, $\int v(|\mathbf{x}|)\mathrm{d}\mathbf{x}$ is the first Born approximation to $8\pi\mu a$ (note that a depends on μ!), this is not in conflict with (2.8). For ‘hard’ potentials on the other hand, the ground state is *highly correlated*, i.e., it is far from being a product of single particle states. The energy is here *mostly kinetic*, because the wave function is very small where the potential is large. These two quite different regimes, the potential energy dominated one and the kinetic energy dominated one, cannot be distinguished by the low density asymptotics of the energy. Whether they behave differently with respect to other phenomena, e.g., Bose–Einstein condensation, is not known at present.

Bogolubov's analysis [7] presupposes the existence of Bose–Einstein condensation. Nevertheless, it is correct (for the energy) for the one-dimensional delta-function Bose gas [48], despite the fact that there is (presumably) no condensation in that case [72]. It turns out that BE condensation is not really needed in order to understand the energy. As we shall see, ‘global’ condensation can be replaced by a ‘local’ condensation on boxes whose size is independent of L. It is this crucial understanding that enables us to prove Theorem 2.1 without having to decide about BE condensation.

An important idea of Dyson was to transform the hard sphere potential into a soft potential at the cost of sacrificing the kinetic energy, i.e., effectively to move from one regime to the other. We shall make use of this idea in our proof of the lower bound below. But first we discuss the simpler upper bound, which relies on other ideas from Dyson's beautiful paper [17].

2.1 Upper Bound

The following generalization of Dyson's upper bound holds [53], [77]:

Theorem 2.2 (Upper bound). *Let* $\rho_1 = (N-1)/L^3$ *and* $b = (4\pi\rho_1/3)^{-1/3}$. *For non-negative potentials* v *and* $b > a$ *the ground state energy of* (2.1) *with periodic boundary conditions satisfies*

$$E_0(N,L)/N \leq 4\pi\mu\rho_1 a \frac{1-\frac{a}{b}+\left(\frac{a}{b}\right)^2+\frac{1}{2}\left(\frac{a}{b}\right)^3}{\left(1-\frac{a}{b}\right)^8} \,. \tag{2.14}$$

Thus in the thermodynamic limit (and for all boundary conditions)

$$\frac{e_0(\rho)}{4\pi\mu\rho a} \leq \frac{1-Y^{1/3}+Y^{2/3}-\frac{1}{2}Y}{(1-Y^{1/3})^8} \,, \tag{2.15}$$

provided $Y = 4\pi\rho a^3/3 < 1$.

Remark. The bound (2.14) holds for potentials with infinite range, provided $b > a$. For potentials of finite range R_0 it can be improved for $b > R_0$ to

$$E_0(N,L)/N \leq 4\pi\mu\rho_1 a \frac{1-\left(\frac{a}{b}\right)^2+\frac{1}{2}\left(\frac{a}{b}\right)^3}{\left(1-\frac{a}{b}\right)^4} \,. \tag{2.16}$$

Proof. We first remark that the expectation value of (2.1) with any trial wave function gives an upper bound to the bosonic ground state energy, even if the trial function is not symmetric under permutations of the variables. The reason is that an absolute ground state of the elliptic differential operator (2.1) (i.e., a ground state without symmetry requirement) is a nonnegative function which can be symmetrized without changing the energy because (2.1) is symmetric under permutations. In other words, the absolute ground state energy is the same as the bosonic ground state energy.

Following [17] we choose a trial function of the following form

$$\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N) = F_1(\mathbf{x}_1)F_2(\mathbf{x}_1,\mathbf{x}_2)\cdots F_N(\mathbf{x}_1,\ldots,\mathbf{x}_N) \,. \tag{2.17}$$

More specifically, $F_1 \equiv 1$ and F_i depends only on the distance of $\mathbf{x}_i$ to its nearest neighbor among the points $\mathbf{x}_1,\ldots,\mathbf{x}_{i-1}$ (taking the periodic boundary into account):

$$F_i(\mathbf{x}_1,\ldots,\mathbf{x}_i) = f(t_i), \quad t_i = \min\left(|\mathbf{x}_i-\mathbf{x}_j|, j=1,\ldots,i-1\right) \,, \tag{2.18}$$

with a function f satisfying

$$0 \leq f \leq 1 \,, \quad f' \geq 0 \,. \tag{2.19}$$

The intuition behind the ansatz (2.17) is that the particles are inserted into the system one at the time, taking into account the particles previously inserted.

While such a wave function cannot reproduce all correlations present in the true ground state, it turns out to capture the leading term in the energy for dilute gases. The form (2.17) is computationally easier to handle than an ansatz of the type $\prod_{i<j} f(|\mathbf{x}_i - \mathbf{x}_j|)$, which might appear more natural in view of the heuristic remarks after (2.13).

The function f is chosen to be

$$f(r) = \begin{cases} f_0(r)/f_0(b) & \text{for } 0 \leq r \leq b\,, \\ 1 & \text{for } r > b\,, \end{cases} \tag{2.20}$$

with $f_0(r) = u_0(r)/r$ the zero energy scattering solution defined by (2.6). The estimates (2.14) and (2.16) are obtained by somewhat lengthy computations similar as in [17], but making use of (2.13). For details we refer to [53] and [77]. □

2.2 Lower Bound

It was explained previously in this section why the lower bound for the bosonic ground state energy of (2.1) is not easy to obtain. The three different length scales (2.12) for bosons will play a role in the proof below.

- The scattering length a.
- The mean particle distance $\rho^{-1/3}$.
- The 'uncertainty principle length' ℓ_c, defined by $\mu\ell_c^{-2} = e_0(\rho)$, i.e., $\ell_c \sim (\rho a)^{-1/2}$.

Our lower bound for $e_0(\rho)$ is as follows.

Theorem 2.3 (Lower bound in the thermodynamic limit). *For a positive potential v with finite range and Y small enough*

$$\frac{e_0(\rho)}{4\pi\mu\rho a} \geq (1 - CY^{1/17}) \tag{2.21}$$

with C a constant. If v does not have finite range, but decreases faster than $1/r^3$ (more precisely, $\int_R^\infty v(r)r^2 \mathrm{d}r < \infty$ for some R) then an analogous bound to (2.21) *holds, but with $CY^{1/17}$ replaced by $o(1)$ as $Y \to 0$.*

It should be noted right away that the error term $-CY^{1/17}$ in (2.21) is of no fundamental significance and is not believed to reflect the true state of affairs. Presumably, it does not even have the right sign. We mention in passing that C can be taken to be 8.9 [77].

As mentioned at the beginning of this section after (2.2), a lower bound on $E_0(N, L)$ for finite N and L is of importance for applications to inhomogeneous gases, and in fact we derive (2.21) from such a bound. We state it in the following way:

Theorem 2.4 (Lower bound in a finite box). *For a positive potential v with finite range there is a $\delta > 0$ such that the ground state energy of* (2.1) *with Neumann boundary conditions satisfies*

$$E_0(N, L)/N \geq 4\pi\mu\rho a \left(1 - C\, Y^{1/17}\right) \tag{2.22}$$

for all N and L with $Y < \delta$ and $L/a > C'Y^{-6/17}$. Here C and C' are positive constants, independent of N and L. (Note that the condition on L/a requires in particular that N must be large enough, $N >$ (const.)$Y^{-1/17}$.) As in Theorem 2.3 such a bound, but possibly with a different error term holds also for potentials v of infinite range that decrease sufficiently fast at infinity.

The first step in the proof of Theorem 2.4 is a generalization of a lemma of Dyson, which allows us to replace v by a 'soft' potential, at the cost of sacrificing kinetic energy and increasing the effective range.

Lemma 2.5. *Let $v(r) \geq 0$ with finite range R_0. Let $U(r) \geq 0$ be any function satisfying $\int U(r) r^2 \mathrm{d}r \leq 1$ and $U(r) = 0$ for $r < R_0$. Let $\mathcal{B} \subset \mathbb{R}^3$ be star shaped with respect to 0 (e.g. convex with $0 \in \mathcal{B}$). Then for all differentiable functions ψ*

$$\int_{\mathcal{B}} \left[\mu|\nabla\psi|^2 + \tfrac{1}{2}v|\psi|^2\right] \geq \mu a \int_{\mathcal{B}} U|\psi|^2 \, . \tag{2.23}$$

Proof. Actually, (2.23) holds with $\mu|\nabla\psi(\mathbf{x})|^2$ replaced by the (smaller) radial kinetic energy, $\mu|\partial\psi(\mathbf{x})/\partial r|^2$, and it suffices to prove the analog of (2.23) for the integral along each radial line with fixed angular variables. Along such a line we write $\psi(\mathbf{x}) = u(r)/r$ with $u(0) = 0$. We consider first the special case when U is a delta-function at some radius $R \geq R_0$, i.e.,

$$U(r) = \frac{1}{R^2}\delta(r - R) \, . \tag{2.24}$$

For such U the analog of (2.23) along the radial line is

$$\int_0^{R_1} \{\mu[u'(r) - (u(r)/r)]^2 + \tfrac{1}{2}v(r)|u(r)|^2\}\mathrm{d}r \geq \begin{cases} 0 & \text{if } R_1 < R \\ \mu a|u(R)|^2/R^2 & \text{if } R \leq R_1 \end{cases} \tag{2.25}$$

where R_1 is the length of the radial line segment in $\mathcal{B}$. The case $R_1 < R$ is trivial, because $\mu|\partial\psi/\partial r|^2 + \frac{1}{2}v|\psi|^2 \geq 0$. (Note that positivity of v is used here.) If $R \leq R_1$ we consider the integral on the left side of (2.25) from 0 to R instead of R_1 and minimize it under the boundary condition that $u(0) = 0$ and $u(R)$ is a fixed constant. Since everything is homogeneous in u we may normalize this value to $u(R) = R - a$. This minimization problem leads to the zero energy scattering equation (2.6). Since v is positive, the solution is a true minimum and not just a stationary point.

Because $v(r) = 0$ for $r > R_0$ the solution, u_0, satisfies $u_0(r) = r - a$ for $r > R_0$. By partial integration,

$$\int_0^R \{\mu[u_0'(r) - (u_0(r)/r)]^2 + \tfrac{1}{2}v(r)|u_0(r)|^2\}\mathrm{d}r = \mu a|R-a|/R \\ \geq \mu a|R-a|^2/R^2 \; . \tag{2.26}$$

But $|R-a|^2/R^2$ is precisely the right side of (2.25) if u satisfies the normalization condition.

This derivation of (2.23) for the special case (2.24) implies the general case, because every U can be written as a superposition of δ-functions, $U(r) = \int R^{-2}\delta(r-R)\,U(R)R^2\mathrm{d}R$, and $\int U(R)R^2\mathrm{d}R \leq 1$ by assumption. □

By dividing Λ for given points $\mathbf{x}_1, \ldots, \mathbf{x}_N$ into Voronoi cells $\mathcal{B}_i$ that contain all points closer to $\mathbf{x}_i$ than to $\mathbf{x}_j$ with $j \neq i$ (these cells are star shaped w.r.t. $\mathbf{x}_i$, indeed convex), the following corollary of Lemma 2.5 can be derived in the same way as the corresponding Eq. (28) in [17].

Corollary 2.6. *For any U as in Lemma 2.5*

$$H_N \geq \mu a W \tag{2.27}$$

with W the multiplication operator

$$W(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \sum_{i=1}^{N} U(t_i) \; , \tag{2.28}$$

where t_i is the distance of $\mathbf{x}_i$ to its nearest neighbor *among the other points $\mathbf{x}_j$, $j = 1, \ldots, N$, i.e.,*

$$t_i(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \min_{j,\, j\neq i} |\mathbf{x}_i - \mathbf{x}_j| \; . \tag{2.29}$$

(Note that t_i has here a slightly different meaning than in (2.18), where it denoted the distance to the nearest neighbor among the $\mathbf{x}_j$ with $j \leq i-1$.)

Dyson considers in [17] a one parameter family of U's that is essentially the same as the following choice, which is convenient for the present purpose:

$$U_R(r) = \begin{cases} 3(R^3 - R_0^3)^{-1} & \text{for } R_0 < r < R \\ 0 & \text{otherwise.} \end{cases} \tag{2.30}$$

We denote the corresponding interaction (2.28) by W_R. For the hard core gas one obtains

$$E(N,L) \geq \sup_R \inf_{(\mathbf{x}_1,\ldots,\mathbf{x}_N)} \mu a W_R(\mathbf{x}_1, \ldots, \mathbf{x}_N) \tag{2.31}$$

where the infimum is over $(\mathbf{x}_1, \ldots, x_N) \in \Lambda^N$ with $|\mathbf{x}_i - \mathbf{x}_j| \geq R_0 = a$, because of the hard core. At fixed R simple geometry gives

$$\inf_{(\mathbf{x}_1,\ldots,\mathbf{x}_N)} W_R(\mathbf{x}_1,\ldots,\mathbf{x}_N) \geq \left(\frac{A}{R^3} - \frac{B}{\rho R^6}\right) \tag{2.32}$$

with certain constants A and B. An evaluation of these constants gives Dyson's bound

$$E(N,L)/N \geq \frac{1}{10\sqrt{2}} 4\pi\mu\rho a \ . \tag{2.33}$$

The main reason this method does not give a better bound is that R must be chosen quite big, namely of the order of the mean particle distance $\rho^{-1/3}$, in order to guarantee that the spheres of radius R around the N points overlap. Otherwise the infimum of W_R will be zero. But large R means that W_R is small. It should also be noted that this method does not work for potentials other than hard spheres: If $|\mathbf{x}_i - \mathbf{x}_j|$ is allowed to be less than R_0, then the right side of (2.31) is zero because $U(r) = 0$ for $r < R_0$.

For these reasons we take another route. We still use Lemma 2.5 to get into the soft potential regime, but we do *not* sacrifice *all* the kinetic energy as in (2.27). Instead we write, for $\varepsilon > 0$

$$H_N = \varepsilon H_N + (1-\varepsilon) H_N \geq \varepsilon T_N + (1-\varepsilon) H_N \tag{2.34}$$

with $T_N = -\sum_i \Delta_i$ and use (2.27) only for the part $(1-\varepsilon)H_N$. This gives

$$H_N \geq \varepsilon T_N + (1-\varepsilon)\mu a W_R \ . \tag{2.35}$$

We consider the operator on the right side from the viewpoint of first order perturbation theory, with εT_N as the unperturbed part, denoted H_0.

The ground state of H_0 in a box of side length L is $\Psi_0(\mathbf{x}_1,\ldots,\mathbf{x}_N) \equiv L^{-3N/2}$ and we denote expectation values in this state by $\langle\cdot\rangle_0$. A computation, cf. Eq. (21) in [62] (see also (3.15)–(3.20)), gives

$$\begin{aligned} 4\pi\rho\left(1-\tfrac{1}{N}\right) &\geq \langle W_R\rangle_0/N \\ &\geq 4\pi\rho\left(1-\tfrac{1}{N}\right)\left(1-\tfrac{2R}{L}\right)^3\left(1+4\pi\rho(R^3-R_0^3)/3\right)^{-1} \ . \end{aligned} \tag{2.36}$$

The rationale behind the various factors is as follows: $(1-\frac{1}{N})$ comes from the fact that the number of pairs is $N(N-1)/2$ and not $N^2/2$, $(1-2R/L)^3$ takes into account the fact that the particles do not interact beyond the boundary of Λ, and the last factor measures the probability to find another particle within the interaction range of the potential U_R for a given particle.

The estimates (2.36) on the first order term look at first sight quite promising, for if we let $L \to \infty$, $N \to \infty$ with $\rho = N/L^3$ fixed, and subsequently take $R \to 0$, then $\langle W_R\rangle_0/N$ converges to $4\pi\rho$, which is just what is desired. But the first order result (2.36) is not a rigorous bound on $E_0(N,L)$, we need *error estimates*, and these will depend on ε, R and L.

We now recall *Temple's inequality* [83] for the expectation values of an operator $H = H_0 + V$ in the ground state $\langle\cdot\rangle_0$ of H_0. It is a simple consequence of the operator inequality

$$(H - E_0)(H - E_1) \geq 0 \tag{2.37}$$

for the two lowest eigenvalues, $E_0 < E_1$, of H and reads

$$E_0 \geq \langle H \rangle_0 - \frac{\langle H^2 \rangle_0 - \langle H \rangle_0^2}{E_1 - \langle H \rangle_0} \tag{2.38}$$

provided $E_1 - \langle H \rangle_0 > 0$. Furthermore, if $V \geq 0$ we may use $E_1 \geq E_1^{(0)} =$ second lowest eigenvalue of H_0 and replace E_1 in (2.38) by $E_1^{(0)}$.

From (2.36) and (2.38) we get the estimate

$$\frac{E_0(N, L)}{N} \geq 4\pi\mu a\rho \left(1 - \mathcal{E}(\rho, L, R, \varepsilon)\right) \tag{2.39}$$

with

$$\begin{aligned} 1 - \mathcal{E}(\rho,&L, R, \varepsilon) \\ &= (1-\varepsilon)\left(1 - \tfrac{1}{\rho L^3}\right)\left(1 - \tfrac{2R}{L}\right)^3 \left(1 + \tfrac{4\pi}{3}\rho(R^3 - R_0^3)\right)^{-1} \\ &\quad \times \left(1 - \frac{\mu a\left(\langle W_R^2 \rangle_0 - \langle W_R \rangle_0^2\right)}{\langle W_R \rangle_0 \left(E_1^{(0)} - \mu a \langle W_R \rangle_0\right)}\right) . \end{aligned} \tag{2.40}$$

To evaluate this further one may use the estimates (2.36) and the bound

$$\langle W_R^2 \rangle_0 \leq 3 \frac{N}{R^3 - R_0^3} \langle W_R \rangle_0 \tag{2.41}$$

which follows from $U_R^2 = 3(R^3 - R_0^3)^{-1} U_R$ together with the Schwarz inequality. A glance at the form of the error term reveals, however, that it is *not* possible here to take the thermodynamic limit $L \to \infty$ with ρ fixed: We have $E_1^{(0)} = \varepsilon\pi^2\mu/L^2$ (this is the kinetic energy of a *single* particle in the first excited state in the box), and the factor $E_1^{(0)} - \mu a \langle W_R \rangle_0$ in the denominator in (2.40) is, up to unimportant constants and lower order terms, $\sim (\varepsilon L^{-2} - a\rho^2 L^3)$. Hence the denominator eventually becomes negative and Temple's inequality looses its validity if L is large enough.

As a way out of this dilemma we divide the big box Λ into cubic *cells* of side length ℓ that is kept *fixed* as $L \to \infty$. The number of cells, L^3/ℓ^3, on the other hand, increases with L. The N particles are distributed among these cells, and we use (2.40), with L replaced by ℓ, N by the particle number, n, in a cell and ρ by n/ℓ^3, to estimate the energy in each cell with *Neumann* conditions on the boundary. For each distribution of the particles we add the contributions from the cells, neglecting interactions across boundaries. Since $v \geq 0$ by assumption, this can only lower the energy. Finally, we minimize over all possible choices of the particle numbers for the various cells adding up to N. The energy obtained in this way is a lower bound to $E_0(N, L)$, because we are effectively allowing discontinuous test functions for the quadratic form given by H_N.

In mathematical terms, the cell method leads to

$$E_0(N,L)/N \geq (\rho\ell^3)^{-1} \inf \sum_{n\geq 0} c_n E_0(n,\ell) \tag{2.42}$$

where the infimum is over all choices of coefficients $c_n \geq 0$ (relative number of cells containing exactly n particles), satisfying the constraints

$$\sum_{n\geq 0} c_n = 1\,, \qquad \sum_{n\geq 0} c_n n = \rho\ell^3\,. \tag{2.43}$$

The minimization problem for the distributions of the particles among the cells would be easy if we knew that the ground state energy $E_0(n,\ell)$ (or a good lower bound to it) were convex in n. Then we could immediately conclude that it is best to have the particles as evenly distributed among the boxes as possible, i.e., c_n would be zero except for the n equal to the integer closest to $\rho\ell^3$. This would give

$$\frac{E_0(N,L)}{N} \geq 4\pi\mu a\rho\,(1-\mathcal{E}(\rho,\ell,R,\varepsilon)) \tag{2.44}$$

i.e., replacement of L in (2.39) by ℓ, which is independent of L. The blow up of $\mathcal{E}$ for $L\to\infty$ would thus be avoided.

Since convexity of $E_0(n,\ell)$ is not known (except in the thermodynamic limit) we must resort to other means to show that $n = O(\rho\ell^3)$ in all boxes. The rescue comes from *superadditivity* of $E_0(n,\ell)$, i.e., the property

$$E_0(n+n',\ell) \geq E_0(n,\ell) + E_0(n',\ell) \tag{2.45}$$

which follows immediately from $v\geq 0$ by dropping the interactions between the n particles and the n' particles. The bound (2.45) implies in particular that for any $n,p\in\mathbb{N}$ with $n\geq p$

$$E_0(n,\ell) \geq [n/p]\,E_0(p,\ell) \geq \frac{n}{2p}E_0(p,\ell) \tag{2.46}$$

since the largest integer $[n/p]$ smaller than n/p is in any case $\geq n/(2p)$.

The way (2.46) is used is as follows: Replacing L by ℓ, N by n and ρ by n/ℓ^3 in (2.39) we have for fixed R and ε

$$E_0(n,\ell) \geq \frac{4\pi\mu a}{\ell^3} n(n-1)K(n,\ell) \tag{2.47}$$

with a certain function $K(n,\ell)$ determined by (2.40). We shall see that K is monotonously decreasing in n, so that if $p\in\mathbb{N}$ and $n\leq p$ then

$$E_0(n,\ell) \geq \frac{4\pi\mu a}{\ell^3} n(n-1)K(p,\ell)\,. \tag{2.48}$$

We now split the sum in (2.42) into two parts. For $n < p$ we use (2.48), and for $n \geq p$ we use (2.46) together with (2.48) for $n = p$. The task is thus to minimize

$$\sum_{n<p} c_n n(n-1) + \tfrac{1}{2} \sum_{n \geq p} c_n n(p-1) \tag{2.49}$$

subject to the constraints (2.43). Putting

$$k := \rho \ell^3 \quad \text{and} \quad t := \sum_{n<p} c_n n \leq k \tag{2.50}$$

we have $\sum_{n \geq p} c_n n = k - t$, and since $n(n-1)$ is convex in n and vanishes for $n = 0$, and $\sum_{n<p} c_n \leq 1$, the expression (2.49) is

$$\geq t(t-1) + \tfrac{1}{2}(k-t)(p-1) \, . \tag{2.51}$$

We have to minimize this for $1 \leq t \leq k$. If $p \geq 4k$ the minimum is taken at $t = k$ and is equal to $k(k-1)$. Altogether we have thus shown that

$$\frac{E_0(N, L)}{N} \geq 4\pi\mu a \rho \left(1 - \frac{1}{\rho \ell^3}\right) K(4\rho\ell^3, \ell) \, . \tag{2.52}$$

What remains is to take a closer look at $K(4\rho\ell^3, \ell)$, which depends on the parameters ε and R besides ℓ, and choose the parameters in an optimal way. From (2.40) and (2.41) we obtain

$$\begin{aligned} K(n, \ell) = {} & (1-\varepsilon)\left(1 - \tfrac{2R}{\ell}\right)^3 \left(1 + \tfrac{4\pi}{3}(R^3 - R_0^3)\right)^{-1} \\ & \times \left(1 - \frac{3}{\pi} \frac{an}{(R^3 - R_0^3)(\pi\varepsilon\ell^{-2} - 4a\ell^{-3} n(n-1))}\right) \, . \end{aligned} \tag{2.53}$$

The estimate (2.47) with this K is valid as long as the denominator in the last factor in (2.53) is ≥ 0, and in order to have a formula for all n we can take 0 as a trivial lower bound in other cases or when (2.47) is negative. As required for (2.48), K is monotonously decreasing in n. We now insert $n = 4\rho\ell^3$ and obtain

$$\begin{aligned} K(4\rho\ell^3, \ell) \geq {} & (1-\varepsilon)\left(1 - \tfrac{2R}{\ell}\right)^3 \left(1 + (\text{const.})Y(\ell/a)^3 (R^3 - R_0^3)/\ell^3\right)^{-1} \\ & \times \left(1 - \frac{\ell^3}{(R^3 - R_0^3)} \frac{(\text{const.})Y}{(\varepsilon(a/\ell)^2 - (\text{const.})Y^2(\ell/a)^3)}\right) \end{aligned} \tag{2.54}$$

with $Y = 4\pi\rho a^3/3$ as before. Also, the factor

$$\left(1 - \frac{1}{\rho\ell^3}\right) = (1 - (\text{const.})Y^{-1}(a/\ell)^3) \tag{2.55}$$

in (2.52) (which is the ratio between $n(n-1)$ and n^2) must not be forgotten. We now make the ansatz

$$\varepsilon \sim Y^{\alpha}, \quad a/\ell \sim Y^{\beta}, \quad (R^3 - R_0^3)/\ell^3 \sim Y^{\gamma} \tag{2.56}$$

with exponents α, β and γ that we choose in an optimal way. The conditions to be met are as follows:

- $\varepsilon(a/\ell)^2 - (\mathrm{const.})Y^2(\ell/a)^3 > 0$. This holds for all small enough Y, provided $\alpha + 5\beta < 2$ which follows from the conditions below.
- $\alpha > 0$ in order that $\varepsilon \to 0$ for $Y \to 0$.
- $3\beta - 1 > 0$ in order that $Y^{-1}(a/\ell)^3 \to 0$ for for $Y \to 0$.
- $1 - 3\beta + \gamma > 0$ in order that $Y(\ell/a)^3(R^3 - R_0^3)/\ell^3 \to 0$ for for $Y \to 0$.
- $1 - \alpha - 2\beta - \gamma > 0$ to control the last factor in (2.54).

Taking

$$\alpha = 1/17\,, \quad \beta = 6/17\,, \quad \gamma = 3/17 \tag{2.57}$$

all these conditions are satisfied, and

$$\alpha = 3\beta - 1 = 1 - 3\beta + \gamma = 1 - \alpha - 2\beta - \gamma = 1/17\,. \tag{2.58}$$

It is also clear that $2R/\ell \sim Y^{\gamma/3} = Y^{1/17}$, up to higher order terms. This completes the proof of Theorems 2.3 and 2.4, for the case of potentials with finite range. By optimizing the proportionality constants in (2.56) one can show that $C = 8.9$ is possible in Theorem 2.3 [77]. The extension to potentials of infinite range but finite scattering length is obtained by approximation by finite range potentials, controlling the change of the scattering length as the cut-off is removed. See Appendix A in [63] and Appendix B in [53] for details. We remark that a slower decrease of the potential than $1/r^3$ implies infinite scattering length. □

The exponents (2.57) mean in particular that

$$a \ll R \ll \rho^{-1/3} \ll \ell \ll (\rho a)^{-1/2}\,, \tag{2.59}$$

whereas Dyson's method required $R \sim \rho^{-1/3}$ as already explained. The condition $\rho^{-1/3} \ll \ell$ is required in order to have many particles in each box and thus $n(n-1) \approx n^2$. The condition $\ell \ll (\rho a)^{-1/2}$ is necessary for a spectral gap $\gg e_0(\rho)$ in Temple's inequality. It is also clear that this choice of ℓ would lead to a far too big energy and no bound for $e_0(\rho)$ if we had chosen Dirichlet instead of Neumann boundary conditions for the cells. But with the latter the method works!

3 The Dilute Bose Gas in 2D

In contrast to the three-dimensional theory, the two-dimensional Bose gas began to receive attention only relatively late. The first derivation of the correct asymptotic formula was, to our knowledge, done by Schick [75] for a gas of hard discs. He found

$$e(\rho) \approx 4\pi\mu\rho|\ln(\rho a^2)|^{-1} . \tag{3.1}$$

This was accomplished by an infinite summation of 'perturbation series' diagrams. Subsequently, a corrected modification of [75] was given in [32]. Positive temperature extensions were given in [73] and in [22]. All this work involved an analysis in momentum space, with the exception of a method due to one of us that works directly in configuration space [44]. Ovchinnikov [68] derived (3.1) by using, basically, the method in [44]. These derivations require several unproven assumptions and are not rigorous.

In two dimensions the scattering length a is defined using the zero energy scattering equation (2.3) but instead of $\psi(r) \approx 1 - a/r$ we now impose the asymptotic condition $\psi(r) \approx \ln(r/a)$. This is explained in the appendix to [63].

Note that in two dimensions the ground state energy could not possibly be $e_0(\rho) \approx 4\pi\mu\rho a$ as in three dimensions because that would be dimensionally wrong. Since $e_0(\rho)$ should essentially be proportional to ρ, there is apparently no room for an a dependence — which is ridiculous! It turns out that this dependence comes about in the $\ln(\rho a^2)$ factor.

One of the intriguing facts about (3.1) is that the energy for N particles is *not equal* to $N(N-1)/2$ times the energy for two particles in the low density limit — as is the case in three dimensions. The latter quantity, $E_0(2, L)$, is, asymptotically for large L, equal to $8\pi\mu L^{-2}\left[\ln(L^2/a^2)\right]^{-1}$. (This is seen in an analogous way as (2.13). The three-dimensional boundary condition $\psi_0(|\mathbf{x}| = R) = 1 - a/R$ is replaced by $\psi_0(|\mathbf{x}| = R) = \ln(R/a)$ and moreover it has to be taken into account that with this normalization $\|\psi_0\|^2 = (\text{volume})(\ln(R/a))^2$ (to leading order), instead of just the volume in the three-dimensional case.) Thus, if the $N(N-1)/2$ rule were to apply, (3.1) would have to be replaced by the much smaller quantity $4\pi\mu\rho\left[\ln(L^2/a^2)\right]^{-1}$. In other words, L, which tends to ∞ in the thermodynamic limit, has to be replaced by the mean particle separation, $\rho^{-1/2}$ in the logarithmic factor. Various poetic formulations of this curious fact have been given, but the fact remains that the non-linearity is something that does not occur in more than two dimensions and its precise nature is hardly obvious, physically. This anomaly is the main reason that the two-dimensional case is not a trivial extension of the three-dimensional one.

Equation (3.1) was proved in [63] for nonnegative, finite range two-body potentials by finding upper and lower bounds of the correct form, using similar ideas as in the previous section for the three-dimensional case. We discuss below the modifications that have to be made in the present two-dimensional case. The restriction to finite range can be relaxed as in three dimensions, but the restriction to nonnegative v cannot be removed in the current state of our methodology. The upper bounds will have relative remainder terms $\mathrm{O}(|\ln(\rho a^2)|^{-1})$ while the lower bound will have remainder $\mathrm{O}(|\ln(\rho a^2)|^{-1/5})$. It is claimed in [32] that the relative error for a hard core gas is negative and $\mathrm{O}(\ln|\ln(\rho a^2)||\ln(\rho a^2)|^{-1})$, which is consistent with our bounds.

The upper bound is derived in complete analogy with the three dimensional case. The function f_0 in the variational ansatz (2.20) is in two dimensions also the zero energy scattering solution — but for 2D, of course. The result is

$$E_0(N,L)/N \leq \frac{2\pi\mu\rho}{\ln(b/a) - \pi\rho b^2}\left(1 + \mathrm{O}([\ln(b/a)]^{-1})\right) . \tag{3.2}$$

The minimum over b of the leading term is obtained for $b = (2\pi\rho)^{-1/2}$. Inserting this in (3.2) we thus obtain

$$E_0(N,L)/N \leq \frac{4\pi\mu\rho}{|\ln(\rho a^2)|}\left(1 + \mathrm{O}(|\ln(\rho a^2)|^{-1})\right) . \tag{3.3}$$

To prove the lower bound the essential new step is to modify Dyson's lemma for 2D. The 2D version of Lemma 2.5 is:

Lemma 3.1. *Let $v(r) \geq 0$ and $v(r) = 0$ for $r > R_0$. Let $U(r) \geq 0$ be any function satisfying*

$$\int_0^\infty U(r)\ln(r/a) r\mathrm{d}r \leq 1 \qquad \text{and} \qquad U(r) = 0 \quad \text{for } r < R_0 . \tag{3.4}$$

Let $\mathcal{B} \subset \mathbb{R}^2$ be star-shaped with respect to 0 (e.g. convex with $0 \in \mathcal{B}$). Then, for all functions ψ in the Sobolev space $H^1(\mathcal{B})$,

$$\int_{\mathcal{B}} \left(\mu|\nabla\psi(\mathbf{x})|^2 + \tfrac{1}{2}v(|\mathbf{x}|)|\psi(\mathbf{x})|^2\right) \mathrm{d}\mathbf{x} \geq \mu \int_{\mathcal{B}} U(|\mathbf{x}|)|\psi(\mathbf{x})|^2 \,\mathrm{d}\mathbf{x} . \tag{3.5}$$

Proof. In polar coordinates, r, θ, one has $|\nabla\psi|^2 \geq |\partial\psi/\partial r|^2$. Therefore, it suffices to prove that for each angle $\theta \in [0, 2\pi)$, and with $\psi(r,\theta)$ denoted simply by $f(r)$,

$$\int_0^{R(\theta)} \left(\mu|\partial f(r)/\partial r|^2 + \tfrac{1}{2}v(r)|f(r)|^2\right) r\mathrm{d}r \geq \mu \int_0^{R(\theta)} U(r)|f(r)|^2 \, r\mathrm{d}r , \tag{3.6}$$

where $R(\theta)$ denotes the distance of the origin to the boundary of $\mathcal{B}$ along the ray θ.

If $R(\theta) \leq R_0$ then (3.6) is trivial because the right side is zero while the left side is evidently nonnegative. (Here, $v \geq 0$ is used.)

If $R(\theta) > R_0$ for some given value of θ, consider the disc $\mathcal{D}(\theta) = \{\mathbf{x} \in \mathbb{R}^2 \,:\, 0 \leq |\mathbf{x}| \leq R(\theta)\}$ centered at the origin in $\mathbb{R}^2$ and of radius $R(\theta)$. Our function f defines a spherically symmetric function, $\mathbf{x} \mapsto f(|\mathbf{x}|)$ on $\mathcal{D}(\theta)$, and (3.6) is equivalent to

$$\int_{\mathcal{D}(\theta)} \left(\mu|\nabla f(|\mathbf{x}|)|^2 + \frac{1}{2}v(|\mathbf{x}|)|f(|\mathbf{x}|)|^2\right) \mathrm{d}\mathbf{x} \geq \mu \int_{\mathcal{D}(\theta)} U(|\mathbf{x}|)|f(|\mathbf{x}|)|^2 \mathrm{d}\mathbf{x} . \tag{3.7}$$

Now choose some $R \in (R_0,\ R(\theta))$ and note that the left side of (3.7) is not smaller than the same quantity with $\mathcal{D}(\theta)$ replaced by the smaller disc $\mathcal{D}_R = \{\mathbf{x} \in \mathbb{R}^2\ :\ 0 \le |\mathbf{x}| \le R\}$. (Again, $v \ge 0$ is used.) We now minimize this integral over $\mathcal{D}_R$, fixing $f(R)$. This minimization problem leads to the zero energy scattering equation. Plugging in the solution and integrating by parts leads to

$$2\pi \int_0^{R(\theta)} \left(\mu|\partial f(r)/\partial r|^2 + \frac{1}{2}v(r)|f(r)|^2\right) r\mathrm{d}r \ge \frac{2\pi\mu}{\ln(R/a)}|f(R)|^2\,. \tag{3.8}$$

The proof is completed by multiplying both sides of (3.8) by $U(R)R\ln(R/a)$ and integrating with respect to R from R_0 to $R(\theta)$. □

As in Corollary 2.6, Lemma 3.1 can be used to bound the many body Hamiltonian H_N from below, as follows:

Corollary 3.2. *For any U as in Lemma 3.1 and any $0 < \varepsilon < 1$*

$$H_N \ge \varepsilon T_N + (1-\varepsilon)\mu W \tag{3.9}$$

with $T_N = -\mu\sum_{i=1}^N \Delta_i$ and

$$W(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \sum_{i=1}^N U\left(\min_{j,\, j\neq i} |\mathbf{x}_i - \mathbf{x}_j|\right)\,. \tag{3.10}$$

For U we choose the following functions, parameterized by $R > R_0$:

$$U_R(r) = \begin{cases} \nu(R)^{-1} & \text{for } R_0 < r < R \\ 0 & \text{otherwise} \end{cases} \tag{3.11}$$

with $\nu(R)$ chosen so that

$$\int_{R_0}^R U_R(r)\ln(r/a) r\,\mathrm{d}r = 1 \tag{3.12}$$

for all $R > R_0$, i.e.,

$$\begin{aligned} \nu(R) &= \int_{R_0}^R \ln(r/a) r\,\mathrm{d}r \\ &= \tfrac{1}{4}\left\{R^2\left(\ln(R^2/a^2)-1\right) - R_0^2\left(\ln(R_0^2/a^2)-1\right)\right\}\,. \end{aligned} \tag{3.13}$$

The nearest neighbor interaction (3.10) corresponding to U_R will be denoted W_R.

As in Sect. 2.2 we shall need estimates on the expectation value, $\langle W_R\rangle_0$, of W_R in the ground state of εT_N of (3.9) with Neumann boundary conditions. This is just the average value of W_R in a hypercube in $\mathbb{R}^{2N}$. Besides the normalization factor $\nu(R)$, the computation involves the volume (area) of the support of U_R, which is

$$A(R) = \pi(R^2 - R_0^2) \ . \tag{3.14}$$

In contrast to the three-dimensional situation the normalization factor $\nu(R)$ is not just a constant (R independent) multiple of $A(R)$; the factor $\ln(r/a)$ in (3.4) accounts for the more complicated expressions in the two-dimensional case. Taking into account that U_R is proportional to the characteristic function of a disc of radius R with a hole of radius R_0, the following inequalities for n particles in a box of side length ℓ are obtained by the same geometric reasoning as lead to (2.36), cf. [62]:

$$\langle W_R\rangle_0 \geq \frac{n}{\nu(R)}\left(1-\tfrac{2R}{\ell}\right)^2\left[1-(1-Q)^{(n-1)}\right] \tag{3.15}$$

$$\langle W_R\rangle_0 \leq \frac{n}{\nu(R)}\left[1-(1-Q)^{(n-1)}\right] \tag{3.16}$$

with

$$Q = A(R)/\ell^2 \tag{3.17}$$

being the relative volume occupied by the support of the potential U_R. Since $U_R^2 = \nu(R)^{-1}U_R$ we also have

$$\langle W_R^2\rangle_0 \leq \frac{n}{\nu(R)}\langle W_R\rangle_0 \ . \tag{3.18}$$

As in [62] we estimate $[1-(1-Q)^{(n-1)}]$ by

$$(n-1)Q \geq \left[1-(1-Q)^{(n-1)}\right] \geq \frac{(n-1)Q}{1+(n-1)Q} \tag{3.19}$$

This gives

$$\langle W_R\rangle_0 \geq \frac{n(n-1)}{\nu(R)}\frac{Q}{1+(n-1)Q} \ , \tag{3.20}$$

$$\langle W_R\rangle_0 \leq \frac{n(n-1)}{\nu(R)}Q \ . \tag{3.21}$$

From Temple's inequality [83] we obtain like in (2.38) the estimate

$$E_0(n,\ell) \geq (1-\varepsilon)\langle W_R\rangle_0\left(1-\frac{\mu\big(\langle W_R^2\rangle_0-\langle W_R\rangle_0^2\big)}{\langle W_R\rangle_0\big(E_1^{(0)}-\mu\langle W_R\rangle_0\big)}\right) \tag{3.22}$$

where

$$E_1^{(0)} = \frac{\varepsilon\mu}{\ell^2} \tag{3.23}$$

is the energy of the lowest excited state of εT_n. This estimate is valid for $E_1^{(0)}/\mu > \langle W_R\rangle_0$, i.e., it is important that ℓ is not too big.

Putting (3.20)–(3.22) together we obtain the estimate

$$E_0(n,\ell) \geq \frac{n(n-1)}{\ell^2}\,\frac{A(R)}{\nu(R)}\,K(n) \tag{3.24}$$

with

$$K(n) = (1-\varepsilon)\frac{(1-\frac{2R}{\ell})^2}{1+(n-1)Q}\left(1-\frac{n}{(\varepsilon\,\nu(R)/\ell^2)-n(n-1)\,Q}\right). \tag{3.25}$$

Note that Q depends on ℓ and R, and K depends on ℓ, R and ε besides n. We have here dropped the term $\langle W_R\rangle_0^2$ in the numerator in (3.22), which is appropriate for the purpose of a lower bound.

We note that K is monotonically decreasing in n, so for a given n we may replace $K(n)$ by $K(p)$ provided $p \geq n$. As explained in the previous section, (2.45)–(2.52), convexity of $n \mapsto n(n-1)$ together with superadditivity of $E_0(n,\ell)$ in n leads, for $p = 4\rho\ell^2$, to an estimate for the energy of N particles in the large box when the side length L is an integer multiple of ℓ:

$$E_0(N,L)/N \geq \frac{\rho A(R)}{\nu(R)}\left(1-\frac{1}{\rho\ell^2}\right)K(4\rho\ell^2) \tag{3.26}$$

with $\rho = N/L^2$.

Let us now look at the conditions on the parameters ε, R and ℓ that have to be met in order to obtain a lower bound with the same leading term as the upper bound (3.3).

From (3.13) we have

$$\frac{A(R)}{\nu(R)} = \frac{4\pi}{(\ln(R^2/a^2)-1)}\left(1-\mathrm{O}((R_0^2/R^2)\ln(R/R_0)\right) \tag{3.27}$$

We thus see that as long as $a < R < \rho^{-1/2}$ the logarithmic factor in the denominator in (3.27) has the right form for a lower bound. Moreover, for Temple's inequality the denominator in the third factor in (3.25) must be positive. With $n = 4\rho\ell^2$ and $\nu(R) \geq (\mathrm{const.})R^2\ln(R^2/a^2)$ for $R \gg R_0$, this condition amounts to

$$(\mathrm{const.})\varepsilon\ln(R^2/a^2)/\ell^2 > \rho^2\ell^4\ . \tag{3.28}$$

The relative error terms in (3.26) that have to be $\ll 1$ are

$$\varepsilon\ , \quad \frac{1}{\rho\ell^2}\ , \quad \frac{R}{\ell}\ , \quad \rho R^2\ , \quad \frac{\rho\ell^4}{\varepsilon R^2\ln(R^2/a^2)}\ . \tag{3.29}$$

We now choose

$$\begin{gathered}\varepsilon \sim |\ln(\rho a^2)|^{-1/5}\ , \qquad \ell \sim \rho^{-1/2}|\ln(\rho a^2)|^{1/10}\ , \\ R \sim \rho^{-1/2}|\ln(\rho a^2)|^{-1/10}\ .\end{gathered} \tag{3.30}$$

Condition (3.28) is satisfied since the left side is $>$ (const.)$|\ln(\rho a^2)|^{3/5}$ and the right side is $\sim |\ln(\rho a^2)|^{2/5}$. The first three error terms in (3.29) are all of the same order, $|\ln(\rho a^2)|^{-1/5}$, the last is $\sim |\ln(\rho a^2)|^{-1/5}(\ln|\ln(\rho a^2)|)^{-1}$. With these choices, (3.26) thus leads to the following:

Theorem 3.3 (Lower bound). *For all N and L large enough such that $L >$ (const.)$\rho^{-1/2}|\ln(\rho a^2)|^{1/10}$ and $N >$ (const.)$|\ln(\rho a^2)|^{1/5}$ with $\rho = N/L^2$, the ground state energy with Neumann boundary condition satisfies*

$$E_0(N,L)/N \geq \frac{4\pi\mu\rho}{|\ln(\rho a^2)|}\left(1 - \mathrm{O}(|\ln(\rho a^2)|^{-1/5})\right) . \tag{3.31}$$

In combination with the upper bound (3.3) this also proves

Theorem 3.4 (Energy at low density in the thermodynamic limit).

$$\lim_{\rho a^2 \to 0} \frac{e_0(\rho)}{4\pi\mu\rho|\ln(\rho a^2)|^{-1}} = 1 \tag{3.32}$$

where $e_0(\rho) = \lim_{N\to\infty} E_0(N, \rho^{-1/2}N^{1/2})/N$. This holds irrespective of boundary conditions.

As in the three-dimensional case, Theorem 3.4 is also valid for an infinite range potential v provided that $v \geq 0$ and for some R we have $\int_R^\infty v(r)r\,\mathrm{d}r < \infty$, which guarantees a finite scattering length.

4 Generalized Poincaré Inequalities

This section contains some lemmas that are of independent mathematical interest, but whose significance for the physics of the Bose gas may not be obvious at this point. They will, however, turn out to be important tools for the discussion of Bose–Einstein condensation (BEC) and superfluidity in the next section.

The classic Poincaré inequality [49] bounds the L^q-norm of a function, f, orthogonal to a given function g in a domain $\mathcal{K}$, in terms of some L^p-norm of its gradient in $\mathcal{K}$. For the proof of BEC we shall need a generalization of this inequality where the estimate is in terms of the gradient of f on a subset $\Omega \subset \mathcal{K}$ and a remainder that tends to zero with the volume of the complement $\Omega^c = \mathcal{K} \setminus \Omega$. For superfluidity it will be necessary to generalize this further by adding a vector potential to the gradient. This is the most complex of the lemmas because the other two can be derived directly from the classical Poincaré inequality using Hölder's inequality. The first lemma is the simplest variant and it is sufficient for the discussion of BEC in the case of a homogeneous gas. In this case the function g can be taken to be the constant function. The same holds for the second lemma, which will be used for the discussion of superfluidity in a homogeneous gas with periodic boundary conditions, but the modification of the gradient requires a more elaborate proof. The last lemma, that will be used for the discussion of BEC in the inhomogeneous case, is again a simple consequence of the classic Poincaré and Hölder inequalities. For a more comprehensive discussion of generalized Poincaré inequalities with further generalizations we refer to [59].

Lemma 4.1 (Generalized Poincaré inequality: Homogeneous case). *Let $\mathcal{K} \subset \mathbb{R}^3$ be a cube of side length L, and define the average of a function $f \in L^1(\mathcal{K})$ by*

$$\langle f \rangle_{\mathcal{K}} = \frac{1}{L^3} \int_{\mathcal{K}} f(\mathbf{x})\, \mathrm{d}\mathbf{x} \,. \tag{4.1}$$

There exists a constant C such that for all measurable sets $\Omega \subset \mathcal{K}$ and all $f \in H^1(\mathcal{K})$ the inequality

$$\int_{\mathcal{K}} |f(\mathbf{x}) - \langle f \rangle_{\mathcal{K}}|^2 \mathrm{d}\mathbf{x} \leq C \left(L^2 \int_{\Omega} |\nabla f(\mathbf{x})|^2 \mathrm{d}\mathbf{x} + |\Omega^c|^{2/3} \int_{\mathcal{K}} |\nabla f(\mathbf{x})|^2 \mathrm{d}\mathbf{x} \right) \tag{4.2}$$

holds. Here $\Omega^c = \mathcal{K} \setminus \Omega$, and $|\cdot|$ denotes the measure of a set.

Proof. By scaling, it suffices to consider the case $L = 1$. Using the usual Poincaré–Sobolev inequality on $\mathcal{K}$ (see [49], Thm. 8.12), we infer that there exists a $C > 0$ such that

$$\begin{aligned} \|f - \langle f \rangle_{\mathcal{K}}\|^2_{L^2(\mathcal{K})} &\leq \tfrac{1}{2} C \|\nabla f\|^2_{L^{6/5}(\mathcal{K})} \\ &\leq C \left(\|\nabla f\|^2_{L^{6/5}(\Omega)} + \|\nabla f\|^2_{L^{6/5}(\Omega^c)} \right) . \end{aligned} \tag{4.3}$$

Applying Hölder's inequality

$$\|\nabla f\|_{L^{6/5}(\Omega)} \leq \|\nabla f\|_{L^2(\Omega)} |\Omega|^{1/3} \tag{4.4}$$

(and the analogue with Ω replaced by Ω^c), we see that (4.2) holds. □

In the next lemma $\mathcal{K}$ is again a cube of side length L, but we now replace the gradient ∇ by

$$\nabla_{\varphi} := \nabla + i(0, 0, \varphi/L) \,, \tag{4.5}$$

where φ is a real parameter, and require periodic boundary conditions on $\mathcal{K}$.

Lemma 4.2 (Generalized Poincaré inequality with a vector potential). *For any $|\varphi| < \pi$ there are constants $c > 0$ and $C < \infty$ such that for all subsets $\Omega \subset \mathcal{K}$ and all functions $f \in H^1(\mathcal{K})$ with periodic boundary conditions on $\mathcal{K}$ the following estimate holds:*

$$\begin{aligned} \|\nabla_{\varphi} f\|^2_{L^2(\Omega)} \geq{}& \frac{\varphi^2}{L^2} \|f\|^2_{L^2(\mathcal{K})} + \frac{c}{L^2} \|f - \langle f \rangle_{\mathcal{K}}\|^2_{L^2(\mathcal{K})} \\ &- C \left(\|\nabla_{\varphi} f\|^2_{L^2(\mathcal{K})} + \frac{1}{L^2} \|f\|^2_{L^2(\mathcal{K})} \right) \left(\frac{|\Omega|^c}{L^3} \right)^{1/2} . \end{aligned} \tag{4.6}$$

Here $|\Omega^c|$ is the volume of $\Omega^c = \mathcal{K} \setminus \Omega$, the complement of Ω in $\mathcal{K}$.

Proof. We shall derive (4.6) from a special form of this inequality that holds for all functions that are orthogonal to the constant function. Namely, for any positive $\alpha < 2/3$ and some constants $c > 0$ and $\widetilde{C} < \infty$ (depending only on α and $|\varphi| < \pi$) we claim that

$$\|\nabla_\varphi h\|^2_{L^2(\Omega)} \geq \frac{\varphi^2 + c}{L^2}\|h\|^2_{L^2(\mathcal{K})} - \widetilde{C}\left(\frac{|\Omega^c|}{L^3}\right)^\alpha \|\nabla_\varphi h\|^2_{L^2(\mathcal{K})}\,, \tag{4.7}$$

provided $\langle 1, h\rangle_{\mathcal{K}} = 0$. (Remark: Equation (4.7) holds also for $\alpha = 2/3$, but the proof is slightly more complicated in that case. See [59].) If (4.7) is known the derivation of (4.6) is easy: For any f, the function $h = f - L^{-3}\langle 1, f\rangle_{\mathcal{K}}$ is orthogonal to 1. Moreover,

$$\begin{aligned}\|\nabla_\varphi h\|^2_{L^2(\Omega)} &= \|\nabla_\varphi h\|^2_{L^2(\mathcal{K})} - \|\nabla_\varphi h\|^2_{L^2(\Omega^c)}\\
&= \|\nabla_\varphi f\|^2_{L^2(\Omega)} - \frac{\varphi^2}{L^2}|\langle L^{-3/2}, f\rangle_{\mathcal{K}}|^2\left(1 + \frac{|\Omega^c|}{L^3}\right)\\
&\quad + 2\frac{\varphi}{L}\mathrm{Re}\,\langle L^{-3/2}, f\rangle_{\mathcal{K}}\langle \nabla_\varphi f, L^{-3/2}\rangle_{\Omega^c}\\
&\leq \|\nabla_\varphi f\|^2_{L^2(\Omega)} - \frac{\varphi^2}{L^2}|\langle L^{-3/2}, f\rangle_{\mathcal{K}}|^2\\
&\quad + \frac{|\varphi|}{L}\left(L\|\nabla_\varphi f\|^2_{L^2(\mathcal{K})} + \frac{1}{L}\|f\|^2_{L^2(\mathcal{K})}\right)\left(\frac{|\Omega^c|}{L^3}\right)^{1/2}\end{aligned} \tag{4.8}$$

and

$$\begin{aligned}\frac{\varphi^2 + c}{L^2}\|h\|^2_{L^2(\mathcal{K})} &= \frac{\varphi^2}{L^2}\left(\|f\|^2_{L^2(\mathcal{K})} - |\langle L^{-3/2}, f\rangle_{\mathcal{K}}|^2\right)\\
&\quad + \frac{c}{L^2}\|f - L^{-3}\langle 1, f\rangle_{\mathcal{K}}\|^2_{L^2(\mathcal{K})}\,.\end{aligned} \tag{4.9}$$

Setting $\alpha = \frac{1}{2}$, using $\|\nabla_\varphi h\|_{L^2(\mathcal{K})} \leq \|\nabla_\varphi f\|_{L^2(\mathcal{K})}$ in the last term in (4.7) and combining (4.7), (4.8) and (4.9) gives (4.6) with $C = |\varphi| + \widetilde{C}$.

We now turn to the proof of (4.7). For simplicity we set $L = 1$. The general case follows by scaling. Assume that (4.7) is false. Then there exist sequences of constants $C_n \to \infty$, functions h_n with $\|h_n\|_{L^2(\mathcal{K})} = 1$ and $\langle 1, h_n\rangle_{\mathcal{K}} = 0$, and domains $\Omega_n \subset \mathcal{K}$ such that

$$\lim_{n\to\infty}\left\{\|\nabla_\varphi h_n\|^2_{L^2(\Omega_n)} + C_n|\Omega_n^c|^\alpha\|\nabla_\varphi h_n\|^2_{L^2(\mathcal{K})}\right\} \leq \varphi^2\,. \tag{4.10}$$

We shall show that this leads to a contradiction.

Since the sequence h_n is bounded in $L^2(\mathcal{K})$ it has a subsequence, denoted again by h_n, that converges weakly to some $h \in L^2(\mathcal{K})$ (i.e., $\langle g, h_n\rangle_{\mathcal{K}} \to \langle g, h\rangle_{\mathcal{K}}$ for all $g \in L^2(\mathcal{K})$). Moreover, by Hölder's inequality the $L^p(\Omega_n^c)$ norm $\|\nabla_\varphi h_n\|_{L^p(\Omega_n^c)} = (\int_{\Omega_n^c}|\nabla_\varphi h(\mathbf{x})|^p \mathrm{d}\mathbf{x})^{1/p}$ is bounded by $|\Omega_n^c|^{\alpha/2}\|\nabla_\varphi h_n\|_{L^2(\mathcal{K})}$ for $p = 2/(\alpha+1)$. From (4.10) we conclude that $\|\nabla_\varphi h_n\|_{L^p(\Omega_n^c)}$ is bounded and also that $\|\nabla_\varphi h_n\|_{L^p(\Omega_n)} \leq \|\nabla_\varphi h_n\|_{L^2(\Omega_n)}$ is bounded. Altogether, $\nabla_\varphi h_n$

is bounded in $L^p(\mathcal{K})$, and by passing to a further subsequence if necessary, we can therefore assume that $\nabla_\varphi h_n$ converges weakly in $L^p(\mathcal{K})$. The same applies to ∇h_n. Since $p = 2/(\alpha+1)$ with $\alpha < 2/3$ the hypotheses of the Rellich–Kondrashov Theorem [49, Thm. 8.9] are fulfilled and consequently h_n converges *strongly* in $L^2(\mathcal{K})$ to h (i.e., $\|h - h_n\|_{L^2(\mathcal{K})} \to 0$). We shall now show that

$$\liminf_{n\to\infty} \|\nabla_\varphi h_n\|^2_{L^2(\Omega_n)} \geq \|\nabla_\varphi h\|^2_{L^2(\mathcal{K})} \,. \tag{4.11}$$

This will complete the proof because the h_n are normalized and orthogonal to 1 and the same holds for h by strong convergence. Hence the right side of (4.11) is necessarily $> \varphi^2$, since for $|\varphi| < \pi$ the lowest eigenvalue of $-\nabla^2_\varphi$, with constant eigenfunction, is non-degenerate. This contradicts (4.10).

Equation (4.11) is essentially a consequence of the weak lower semicontinuity of the L^2 norm, but the dependence on Ω_n leads to a slight complication. First, (4.10) and $C_n \to \infty$ clearly imply that $|\Omega_n^c| \to 0$, because $\|\nabla_\varphi h_n\|^2_{L^2(\mathcal{K})} > \varphi^2$. By choosing a subsequence we may assume that $\sum_n |\Omega_n^c| < \infty$. For some fixed N let $\widetilde{\Omega}_N = \mathcal{K} \setminus \cup_{n\geq N} \Omega_n^c$. Then $\tilde{\Omega}_N \subset \Omega_n$ for $n \geq N$. Since $\|\nabla_\varphi h_n\|^2_{L^2(\Omega_n)}$ is bounded, $\nabla_\varphi h_n$ is also bounded in $L^2(\widetilde{\Omega}_N)$ and a subsequence of it converges weakly in $L^2(\widetilde{\Omega}_N)$ to $\nabla_\varphi h$. Hence

$$\liminf_{n\to\infty} \|\nabla_\varphi h_n\|^2_{L^2(\Omega_n)} \geq \liminf_{n\to\infty} \|\nabla_\varphi h_n\|^2_{L^2(\widetilde{\Omega}_N)} \geq \|\nabla_\varphi h\|^2_{L^2(\widetilde{\Omega}_N)} \,. \tag{4.12}$$

Since $\widetilde{\Omega}_N \subset \widetilde{\Omega}_{N+1}$ and $\cup_N \widetilde{\Omega}_N = \mathcal{K}$ (up to a set of measure zero), we can now let $N \to \infty$ on the right side of (4.12). By monotone convergence this converges to $\|\nabla_\varphi h\|^2_{L^2(\mathcal{K})}$. This proves (4.11) which, as remarked above, contradicts (4.10). □

The last lemma is a simple generalization of Lemma 4.1 with $\mathcal{K} \subset \mathbb{R}^m$ a bounded and connected set that is sufficiently nice so that the Poincaré–Sobolev inequality (see [49, Thm. 8.12]) holds on $\mathcal{K}$. In particular, this is the case if $\mathcal{K}$ satisfies the cone property [49] (e.g. if $\mathcal{K}$ is a rectangular box or a cube). Moreover, the constant function on $\mathcal{K}$ is here replaced by a more general bounded function.

Lemma 4.3 (Generalized Poincaré inequality: Inhomog. case). *For $d \geq 2$ let $\mathcal{K} \subset \mathbb{R}^d$ be as explained above, and let h be a bounded function with $\int_\mathcal{K} h = 1$. There exists a constant C (depending only on $\mathcal{K}$ and h) such that for all measurable sets $\Omega \subset \mathcal{K}$ and all $f \in H^1(\mathcal{K})$ with $\int_\mathcal{K} fh\,\mathrm{d}\mathbf{x} = 0$, the inequality*

$$\int_\mathcal{K} |f(\mathbf{x})|^2 \mathrm{d}\mathbf{x} \leq C \left(\int_\Omega |\nabla f(\mathbf{x})|^2 \mathrm{d}\mathbf{x} + \left(\frac{|\Omega^c|}{|\mathcal{K}|} \right)^{2/d} \int_\mathcal{K} |\nabla f(\mathbf{x})|^2 \mathrm{d}\mathbf{x} \right) \tag{4.13}$$

holds. Here $|\cdot|$ denotes the measure of a set, and $\Omega^c = \mathcal{K} \setminus \Omega$.

Proof. By the usual Poincaré–Sobolev inequality on $\mathcal{K}$ (see [49, Thm. 8.12]),

$$\begin{aligned} \|f\|^2_{L^2(\mathcal{K})} &\leq \tilde{C}\|\nabla f\|^2_{L^{2d/(d+2)}(\mathcal{K})} \\ &\leq 2\tilde{C}\left(\|\nabla f\|^2_{L^{2d/(d+2)}(\Omega)} + \|\nabla f\|^2_{L^{2d/(d+2)}(\Omega^c)}\right) , \end{aligned} \tag{4.14}$$

if $d \geq 2$ and $\int_{\mathcal{K}} fh = 0$. Applying Hölder's inequality

$$\|\nabla f\|_{L^{2d/(d+2)}(\Omega)} \leq \|\nabla f\|_{L^2(\Omega)}|\Omega|^{1/d} \tag{4.15}$$

(and the analogue with Ω replaced by Ω^c), we see that (4.6) holds with $C = 2|\mathcal{K}|^{2/d}\tilde{C}$. □

5 Bose–Einstein Condensation and Superfluidity for Homogeneous Gases

5.1 Bose–Einstein Condensation

Bose–Einstein condensation (BEC) is the phenomenon of a macroscopic occupation of a single one-particle quantum state, discovered by Einstein for thermal equilibrium states of an ideal Bose gas at sufficiently low temperatures [20]. We are here concerned with interacting Bose gases, where the question of the existence of BEC is highly nontrivial even for the ground state. Due to the interaction the many body ground state is not a product of one-particle states but the concept of a macroscopic occupation of a single state acquires a precise meaning through the *one-particle density* matrix. Given the normalized ground state wave function this is the operator on $L^2(\mathbb{R}^d)$ ($d = 2$ or 3) given by the kernel

$$\gamma(\mathbf{x}, \mathbf{x}') = N \int \Psi_0(\mathbf{x}, \mathbf{X})\Psi_0(\mathbf{x}', \mathbf{X})\mathrm{d}\mathbf{X} , \tag{5.1}$$

where we introduced the short hand notation

$$\mathbf{X} = (\mathbf{x}_2, \ldots, \mathbf{x}_N) \qquad \text{and} \quad \mathrm{d}\mathbf{X} = \prod_{j=2}^{N} \mathrm{d}\mathbf{x}_j . \tag{5.2}$$

Then $\int \gamma(\mathbf{x}, \mathbf{x})\mathrm{d}\mathbf{x} = \mathrm{Tr}\,[\gamma] = N$. BEC in the ground state means, by definition, that this operator has an eigenvalue of order N in the thermodynamic limit. Since γ is a positive kernel and, hopefully, translation invariant in the thermodynamic limit, the eigenfunction belonging to the largest eigenvalue must be the constant function $L^{-d/2}$. Therefore, another way to say that there is BEC in the ground state is that

$$\frac{1}{L^d}\int\int \gamma(\mathbf{x}, \mathbf{y})\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y} = \mathrm{O}(N) \tag{5.3}$$

as $N \to \infty$, $L \to \infty$ with N/L^d fixed; more precisely (5.3) requires that there is a $c > 0$ such that the left side is $> cN$ for all large N. This is also referred to as *off-diagonal long range order*. Unfortunately, this is something that is frequently invoked but has so far never been proved for many body Hamiltonians with genuine interactions — except for one special case: hard core bosons on a lattice at half-filling (i.e., N = half the number of lattice sites). The proof is in [38] and [19].

The problem remains open after more than 75 years since the first investigations on the Bose gas [9, 20]. Our construction in Sect. 2 shows that (in 3D) BEC exists on a length scale of order $\rho^{-1/3}Y^{-1/17}$ which, unfortunately, is not a 'thermodynamic' length like volume$^{1/3}$. The same remark applies to the 2D case of Sect. 3, where BEC is proved over a length scale $\rho^{-1/10}|\ln(\rho a^2)|^{1/10}$.

In a certain limit, however, one can prove (5.3), as has been shown in [51]. In this limit the interaction potential v is varied with N so that the ratio a/L of the scattering length to the box length is of order $1/N$, i.e., the parameter Na/L is kept fixed. Changing a with N can be done by scaling, i.e., we write

$$v(|\mathbf{x}|) = \frac{1}{a^2} v_1(|\mathbf{x}|/a) \tag{5.4}$$

for some v_1 having scattering length 1, and vary a while keeping v_1 fixed. It is easily checked that the v so defined has scattering length a. It is important to note that, in the limit considered, a tends to zero (as $N^{-2/3}$ since $L = (N/\rho)^{1/3} \sim N^{1/3}$ for ρ fixed), and v becomes a *hard* potential of *short* range. This is the *opposite* of the usual mean field limit where the strength of the potential goes to zero while its range tends to infinity.

We shall refer to this as the *Gross–Pitaevskii (GP) limit* since Na/L will turn out to be the natural interaction parameter for inhomogeneous Bose gases confined in traps, that are described by the Gross–Pitaevskii equation discussed in Sects. 6 and 7. Its significance for a homogeneous gas can also be seen by noting that Na/L is the ratio of ρa to $1/L^2$, i.e., in the GP limit the interaction energy per particle is of the same order of magnitude as the energy gap in the box, so that the interaction is still clearly visible, even though $a \to 0$. Note that $\rho a^3 \sim N^{-2}$ in the GP limit, so letting $N \to \infty$ with ρ fixed and Na/L fixed can be regarded as a *simultaneous thermodynamic and low density limit*. For simplicity, we shall here treat only the 3D case.

Theorem 5.1 (BEC in a dilute limit). *Assume that, as $N \to \infty$, $\rho = N/L^3$ and $g = Na/L$ stay fixed, and impose either periodic or Neumann boundary conditions for H. Then*

$$\lim_{N\to\infty} \frac{1}{N}\frac{1}{L^3}\int\int \gamma(\mathbf{x},\mathbf{y})\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y} = 1\ . \tag{5.5}$$

The reason we do not deal with Dirichlet boundary conditions at this point should be clear from the discussion preceding the theorem: There would be an additional contribution $\sim 1/L^2$ to the energy, i.e. of the same order as the interaction energy, and the system would not be homogeneous any more. Dirichlet boundary conditions can, however, be treated with the methods of Sect. 7.

By scaling, the limit in Theorem 5.1 is equivalent to considering a Bose gas in a *fixed box* of side length $L = 1$, and keeping Na fixed as $N \to \infty$, i.e., $a \sim 1/N$. The ground state energy of the system is then, asymptotically, $N \times 4\pi Na$, and Theorem 5.1 implies that the one-particle reduced density matrix γ of the ground state converges, after division by N, to the projection onto the constant function. An analogous result holds true for inhomogeneous systems as will be discussed in Sect. 7.

The proof of Theorem 5.1 has two main ingredients. One is *localization of the energy* that is stated as Lemma 5.2 below. This lemma is a refinement of the energy estimates of Sect. 2.2 and says essentially that the kinetic energy of the ground state is concentrated in a subset of configuration space where at least one pair of particles is close together and whose volume tends to zero as $a \to 0$. The other is the generalized Poincaré inequality, Lemma 4.1 from which one deduces that the one particle density matrix is approximately constant if the kinetic energy is localized in a small set.

The localization lemma will be proved in a slightly more general version that is necessary for Theorem 5.1, namely with the gradient ∇ replaced by $\nabla_\varphi = \nabla + i(0, 0, \varphi/L)$, cf. (4.5). We denote by H'_N the corresponding many-body Hamiltonian (2.1) with ∇_φ in place of ∇. This generalization will be used in the subsequent discussion of superfluidity, but a reader who wishes to focus on Theorem 5.1 only can simply ignore the φ and the reference to the diamagnetic inequality in the proof. We denote the gradient with respect to $\mathbf{x}_1$ by ∇_1, and the corresponding modified operator by $\nabla_{1,\varphi}$.

Lemma 5.2 (Localization of energy). *Let $\mathcal{K}$ be a box of side length L. For all symmetric, normalized wave functions $\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N)$ with periodic boundary conditions on $\mathcal{K}$, and for $N \geq Y^{-1/17}$,*

$$\begin{aligned} \frac{1}{N}\langle \Psi, H'_N \Psi\rangle \geq \left(1 - \mathrm{const.}\, Y^{1/17}\right) \\ \times \left(4\pi\mu\rho a + \mu \int_{\mathcal{K}^{N-1}} \mathrm{d}\mathbf{X} \int_{\Omega_\mathbf{X}} \mathrm{d}\mathbf{x}_1 \left|\nabla_{1,\varphi}\Psi(\mathbf{x}_1, \mathbf{X})\right|^2\right), \end{aligned} \tag{5.6}$$

where $\mathbf{X} = (\mathbf{x}_2, \dots, \mathbf{x}_N)$, $\mathrm{d}\mathbf{X} = \prod_{j=2}^N \mathrm{d}\mathbf{x}_j$, *and*

$$\Omega_\mathbf{X} = \left\{\mathbf{x}_1 : \min_{j\geq 2} |\mathbf{x}_1 - \mathbf{x}_j| \geq R\right\} \tag{5.7}$$

with $R = aY^{-5/17}$.

Proof. Since Ψ is symmetric, the left side of (5.6) can be written as

$$\int_{\mathcal{K}^{N-1}} \mathrm{d}\mathbf{X} \int_{\mathcal{K}} \mathrm{d}\mathbf{x}_1 \left[\mu\left|\nabla_{1,\varphi}\Psi(\mathbf{x}_1, \mathbf{X})\right|^2 + \tfrac{1}{2}\sum_{j\geq 2} v(|\mathbf{x}_1 - \mathbf{x}_j|)|\Psi(\mathbf{x}_1, \mathbf{X})|^2\right]. \tag{5.8}$$

For any $\varepsilon > 0$ and $R > 0$ this is

$$\geq \varepsilon T + (1-\varepsilon)(T^{\text{in}} + I) + (1-\varepsilon)T_\varphi^{\text{out}} \,, \tag{5.9}$$

with

$$T = \mu \int_{\mathcal{K}^{N-1}} \mathrm{d}\mathbf{X} \int_{\mathcal{K}} \mathrm{d}\mathbf{x}_1 \big|\nabla_1 |\Psi(\mathbf{x}_1, \mathbf{X})|\big|^2 \,, \tag{5.10}$$

$$T^{\text{in}} = \mu \int_{\mathcal{K}^{N-1}} \mathrm{d}\mathbf{X} \int_{\Omega_{\mathbf{X}}^c} \mathrm{d}\mathbf{x}_1 \big|\nabla_1 |\Psi(\mathbf{x}_1, \mathbf{X})|\big|^2 \,, \tag{5.11}$$

$$T_\varphi^{\text{out}} = \mu \int_{\mathcal{K}^{N-1}} \mathrm{d}\mathbf{X} \int_{\Omega_{\mathbf{X}}} \mathrm{d}\mathbf{x}_1 \big|\nabla_{1,\varphi} \Psi(\mathbf{x}_1, \mathbf{X})\big|^2 \,, \tag{5.12}$$

and

$$I = \tfrac{1}{2} \int_{\mathcal{K}^{N-1}} \mathrm{d}\mathbf{X} \int_{\mathcal{K}} \mathrm{d}\mathbf{x}_1 \sum_{j \geq 2} v(|\mathbf{x}_1 - \mathbf{x}_j|) |\Psi(\mathbf{x}_1, \mathbf{X})|^2 \,. \tag{5.13}$$

Here

$$\Omega_{\mathbf{X}}^c = \{\mathbf{x}_1 : \; |\mathbf{x}_1 - \mathbf{x}_j| < R \text{ for some } j \geq 2\} \tag{5.14}$$

is the complement of $\Omega_{\mathbf{X}}$, and the diamagnetic inequality [49] $|\nabla_\varphi f(\mathbf{x})|^2 \geq \big|\nabla |f(\mathbf{x})|\big|^2$ has been used. The proof is completed by using the estimates used for the proof of Theorem 2.4 in particular (2.52) and (2.54)–(2.57), which tell us that for $\varepsilon = Y^{1/17}$ and $R = aY^{-5/17}$

$$\varepsilon T + (1-\varepsilon)(T^{\text{in}} + I) \geq \big(1 - \text{const.}\, Y^{1/17}\big) 4\pi\mu\rho a \tag{5.15}$$

as long as $N \geq Y^{-1/17}$. □

Proof (Theorem 5.1). We combine Lemma 5.2 (with $\varphi = 0$ and hence $H'_N = H_N$) with Lemma 4.1 that gives a lower bound to the second term on the right side of (5.6). We thus infer that, for any symmetric Ψ with $\langle \Psi, \Psi \rangle = 1$ and for N large enough,

$$\begin{aligned} &\frac{1}{N} \langle \Psi, H_N \Psi \rangle \big(1 - \text{const.}\, Y^{1/17}\big)^{-1} \\ &\quad \geq 4\pi\mu\rho a - C Y^{1/17} \Big(\frac{1}{L^2} - \frac{1}{N} \big\langle \Psi, \textstyle\sum_j \nabla_j^2 \Psi \big\rangle \Big) \\ &\qquad + \frac{c}{L^2} \int_{\mathcal{K}^{N-1}} \mathrm{d}\mathbf{X} \int_{\mathcal{K}} \mathrm{d}\mathbf{x}_1 \Big| \Psi(\mathbf{x}_1, \mathbf{X}) - L^{-3} \big[\textstyle\int_{\mathcal{K}} \mathrm{d}\mathbf{x} \Psi(\mathbf{x}, \mathbf{X}) \big] \Big|^2 \,, \end{aligned} \tag{5.16}$$

where we used that $|\Omega^c| \leq \frac{4\pi}{3} N R^3 = \text{const.}\, L^3 Y^{2/17}$. Since the kinetic energy, divided by N, is certainly bounded independent of N, as the upper bound (2.14) shows, and since the upper and the lower bound to E_0 agree in the limit considered, the positive last term in (5.16) has to vanish in the limit. I.e., we get that for the ground state wave function Ψ_0 of H_N

$$\lim_{N \to \infty} \int_{\mathcal{K}^{N-1}} \mathrm{d}\mathbf{X} \int_{\mathcal{K}} \mathrm{d}\mathbf{x}_1 \Big| \Psi_0(\mathbf{x}_1, \mathbf{X}) - L^{-3} \big[\textstyle\int_{\mathcal{K}} \mathrm{d}\mathbf{x} \Psi_0(\mathbf{x}, \mathbf{X}) \big] \Big|^2 = 0 \,. \tag{5.17}$$

This proves (5.5), since

$$\int_{\mathcal{K}^{N-1}} \mathrm{d}\mathbf{X} \int_{\mathcal{K}} \mathrm{d}\mathbf{x}_1 \Big| \Psi_0(\mathbf{x}_1, \mathbf{X}) - L^{-3} \big[\textstyle\int_{\mathcal{K}} \mathrm{d}\mathbf{x} \Psi_0(\mathbf{x}, \mathbf{X}) \big] \Big|^2 \\ = 1 - \frac{1}{NL^3} \int_{\mathcal{K}\times\mathcal{K}} \gamma(\mathbf{x}, \mathbf{x}') \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{x}' \,. \quad (5.18)$$

□

5.2 Superfluidity

The phenomenological two-fluid model of superfluidity (see, e.g., [84]) is based on the idea that the particle density ρ is composed of two parts, the density ρ_{s} of the inviscid superfluid and the normal fluid density ρ_{n}. If an external velocity field is imposed on the fluid (for instance by moving the walls of the container) only the viscous normal component responds to the velocity field, while the superfluid component stays at rest. In accord with these ideas the superfluid density in the ground state is often defined as follows [34]: Let E_0 denote the ground state energy of the system in the rest frame and E_0' the ground state energy, measured in the moving frame, when a velocity field $\mathbf{v}$ is imposed. Then for small $\mathbf{v}$

$$\frac{E_0'}{N} = \frac{E_0}{N} + (\rho_{\mathrm{s}}/\rho)\tfrac{1}{2} m \mathbf{v}^2 + O(|\mathbf{v}|^4) \quad (5.19)$$

where N is the particle number and m the particle mass. At positive temperatures the ground state energy should be replaced by the free energy. (Remark: It is important here that (5.19) holds uniformly for all large N; i.e., that the error term $O(|\mathbf{v}|^4)$ can be bounded independently of N. For fixed N and a finite box, (5.19) with $\rho_{\mathrm{s}}/\rho = 1$ always holds for a Bose gas with an arbitrary interaction if $\mathbf{v}$ is small enough, owing to the discreteness of the energy spectrum.[2]) There are other definitions of the superfluid density that may lead to different results [74], but this is the one we shall use here and shall not dwell on this issue since it is not clear that there is a "one-size-fits-all" definition of superfluidity. For instance, in the definition we use here the ideal Bose gas is a perfect superfluid in its ground state, whereas the definition of Landau in terms of a linear dispersion relation of elementary excitations would indicate otherwise. Our main result is that with the definition adopted here there

[2] The ground state with $\mathbf{v} = 0$ remains an eigenstate of the Hamiltonian with arbitrary $\mathbf{v}$ (but not necesssarily a ground state) since its total momentum is zero. Its energy is $\frac{1}{2} m N \mathbf{v}^2$ above the ground state energy for $\mathbf{v} = 0$. Since in a finite box the spectrum of the Hamiltonian for arbitrary $\mathbf{v}$ is discrete and the energy gap above the ground state is bounded away from zero for $\mathbf{v}$ small, the ground state for $\mathbf{v} = 0$ is at the same time the ground state of the Hamiltonian with $\mathbf{v}$ if $\frac{1}{2} m N \mathbf{v}^2$ is smaller than the gap.

is 100% superfluidity in the ground state of a 3D Bose gas in the GP limit explained in the previous subsection.

One of the unresolved issues in the theory of superfluidity is its relation to Bose–Einstein condensation (BEC). It has been argued that in general neither condition is necessary for the other (c.f., e.g., [35, 2, 41]), but in the case considered here, i.e., the GP limit of a 3D gas, we show that 100% BEC into the constant wave function (in the rest frame) prevails even if an external velocity field is imposed. A simple example illustrating the fact that BEC is not necessary for superfluidity is the 1D hard-core Bose gas. This system is well known to have a spectrum like that of an ideal Fermi gas [24] (see also Sect. 8), and it is easy to see that it is superfluid in its ground state in the sense of (5.19). On the other hand, it has no BEC [43, 72]. The definition of the superfluid velocity as the gradient of the phase of the condensate wave function [34, 4] is clearly not applicable in such cases.

We consider a Bose gas with the Hamiltonian (2.1) in a box $\mathcal{K}$ of side length L, assuming periodic boundary conditions in all three coordinate directions. Imposing an external velocity field $\mathbf{v} = (0, 0, \pm|\mathbf{v}|)$ means that the momentum operator $\mathbf{p} = -i\hbar\nabla$ is replaced by by $\mathbf{p} - m\mathbf{v}$, retaining the periodic boundary conditions. The Hamiltonian in the moving frame is thus

$$H'_N = -\mu \sum_{j=1}^{N} \nabla_{j,\varphi}^2 + \sum_{1 \le i < j \le N} v(|\mathbf{x}_i - \mathbf{x}_j|) \,, \tag{5.20}$$

where $\nabla_{j,\varphi} = \nabla_j + i(0, 0, \varphi/L)$ and the dimensionless phase φ is connected to the velocity $\mathbf{v}$ by

$$\varphi = \frac{\pm|\mathbf{v}|Lm}{\hbar} \,. \tag{5.21}$$

Let $E_0(N, a, \varphi)$ denote the ground state energy of (5.20) with periodic boundary conditions. Obviously it is no restriction to consider only the case $-\pi \le \varphi \le \pi$, since E_0 is periodic in φ with period 2π (see Remark 1 below). For Ψ_0 the ground state of H'_N, let γ_N be its one-particle reduced density matrix. We are interested in the *Gross–Pitaevskii* (GP) limit $N \to \infty$ with Na/L fixed. We also fix the box size L. This means that a should vary like $1/N$ which, as explained in the previous subsection, can be achieved by writing $v(r) = a^{-2} v_1(r/a)$, where v_1 is a fixed potential with scattering length 1, while a changes with N.

Theorem 5.3 (Superfluidity and BEC of homogeneous gas).
For $|\varphi| \le \pi$

$$\lim_{N\to\infty} \frac{E_0(N, a, \varphi)}{N} = 4\pi\mu a\rho + \mu\frac{\varphi^2}{L^2} \tag{5.22}$$

in the limit $N \to \infty$ *with* Na/L *and* L *fixed. Here* $\rho = N/L^3$, *so* $a\rho$ *is fixed too. In the same limit, for* $|\varphi| < \pi$,

$$\lim_{N\to\infty} \frac{1}{N}\, \gamma_N(\mathbf{x}, \mathbf{x}') = \frac{1}{L^3} \tag{5.23}$$

in trace class norm, i.e., $\lim_{N\to\infty} \mathrm{Tr}\left[\,\left|\gamma_N/N - |L^{-3/2}\rangle\langle L^{-3/2}|\,\right|\,\right] = 0$.

Note that, by the definition (5.19) of ρ_s and (5.21), (5.22) means that $\rho_s = \rho$, i.e., there is 100% superfluidity. For $\varphi = 0$, (5.22) follows from (2.8), while (5.23) for $\varphi = 0$ is the BEC of Theorem 5.1.[3]

Remarks. 1. By a unitary gauge transformation,

$$\big(U\Psi\big)(\mathbf{x}_1,\ldots,\mathbf{x}_N) = \mathrm{e}^{\mathrm{i}\varphi(\sum_i z_i)/L}\,\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N)\,, \tag{5.24}$$

the passage from (2.1) to (5.20) is equivalent to replacing periodic boundary conditions in a box by the *twisted boundary condition*

$$\Psi(\mathbf{x}_1 + (0,0,L), \mathbf{x}_2,\ldots,\mathbf{x}_N) = \mathrm{e}^{\mathrm{i}\varphi}\Psi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N) \tag{5.25}$$

in the direction of the velocity field, while retaining the original Hamiltonian (2.1).

2. The criterion $|\varphi| \leq \pi$ means that $|\mathbf{v}| \leq \pi\hbar/(mL)$. The corresponding energy $\frac{1}{2}m(\pi\hbar/(mL))^2$ is the gap in the excitation spectrum of the one-particle Hamiltonian in the finite-size system.

3. The reason that we have to restrict ourselves to $|\varphi| < \pi$ in the second part of Theorem 5.3 is that for $|\varphi| = \pi$ there are two ground states of the operator $(\nabla + \mathrm{i}\boldsymbol{\varphi}/L)^2$ with periodic boundary conditions. All we can say in this case is that there is a subsequence of γ_N that converges to a density matrix of rank ≤ 2, whose range is spanned by these two functions

Proof (Theorem 5.3). As in the proof of Theorem 5.1 we combine the localization Lemma 5.2, this time with $\varphi \neq 0$, and a generalized Poincaré inequality, this time Lemma 4.2. We thus infer that, for any symmetric Ψ with $\langle\Psi,\Psi\rangle = 1$ and for N large enough,

$$\begin{aligned} &\frac{1}{N}\langle\Psi, H'_N\Psi\rangle\big(1 - \mathrm{const.}\,Y^{1/17}\big)^{-1} \\ &\quad\geq 4\pi\mu\rho a + \mu\frac{\varphi^2}{L^2} - CY^{1/17}\Big(\frac{1}{L^2} - \frac{1}{N}\big\langle\Psi, \textstyle\sum_j \nabla^2_{j,\varphi}\Psi\big\rangle\Big) \\ &\qquad + \frac{c}{L^2}\int_{\mathcal{K}^{N-1}}\mathrm{d}\mathbf{X}\int_{\mathcal{K}}\mathrm{d}\mathbf{x}_1\,\Big|\Psi(\mathbf{x}_1,\mathbf{X}) - L^{-3}\big[\textstyle\int_{\mathcal{K}}\mathrm{d}\mathbf{x}\,\Psi(\mathbf{x},\mathbf{X})\big]\Big|^2\,, \end{aligned} \tag{5.26}$$

where we used that $|\Omega^c| \leq \frac{4\pi}{3}NR^3 = \mathrm{const.}\,L^3Y^{2/17}$. From this we can infer two things. First, since the kinetic energy, divided by N, is certainly bounded independently of N, as the upper bound shows, we get that

$$\liminf_{N\to\infty}\frac{E_0(N,a,\varphi)}{N} \geq 4\pi\mu\rho a + \mu\frac{\varphi^2}{L^2} \tag{5.27}$$

[3] The convention in Theorem 5.1, where ρ and Na/L stay fixed, is different from the one employed here, where L and Na/L are fixed, but these two conventions are clearly equivalent by scaling.

for any $|\varphi| < \pi$. By continuity this holds also for $|\varphi| = \pi$, proving (5.22). (To be precise, $E_0/N - \mu\varphi^2 L^{-2}$ is concave in φ, and therefore stays concave, and in particular continuous, in the limit $N \to \infty$.) Secondly, since the upper and the lower bounds to E_0 agree in the limit considered, the positive last term in (5.16) has to vanish in the limit. I.e., we get that for the ground state wave function Ψ_0 of H'_N

$$\lim_{N\to\infty} \int_{\mathcal{K}^{N-1}} \mathrm{d}\mathbf{X} \int_{\mathcal{K}} \mathrm{d}\mathbf{x}_1 \left| \Psi_0(\mathbf{x}_1, \mathbf{X}) - L^{-3} \left[\int_{\mathcal{K}} \mathrm{d}\mathbf{x}\, \Psi_0(\mathbf{x}, \mathbf{X}) \right] \right|^2 = 0 \,. \tag{5.28}$$

Using again (5.18), this proves (5.23) in a weak sense. As explained in [51, 52], this suffices for the convergence $N^{-1}\gamma_N \to |L^{-3/2}\rangle\langle L^{-3/2}|$ in trace class norm. □

Theorem 5.3 can be generalized in various ways to a physically more realistic setting, for example replacing the periodic box by a cylinder centered at the origin. We shall comment on such extensions at the end of Sect. 7.

6 Gross–Pitaevskii Equation for Trapped Bosons

In the recent experiments on Bose condensation (see, e.g., [39]), the particles are confined at very low temperatures in a 'trap' where the particle density is *inhomogeneous*, contrary to the case of a large 'box', where the density is essentially uniform. We model the trap by a slowly varying confining potential V, with $V(\mathbf{x}) \to \infty$ as $|\mathbf{x}| \to \infty$. The Hamiltonian becomes

$$H = \sum_{i=1}^{N} \{-\mu\Delta_i + V(\mathbf{x}_i)\} + \sum_{1\le i<j\le N} v(|\mathbf{x}_i - \mathbf{x}_j|) \,. \tag{6.1}$$

Shifting the energy scale if necessary we can assume that V is nonnegative. The ground state energy, $\hbar\omega$, of $-\mu\Delta + V(\mathbf{x})$ is a natural energy unit and the corresponding length unit, $\sqrt{\hbar/(m\omega)} = \sqrt{2\mu/(\hbar\omega)} \equiv L_{\mathrm{osc}}$, is a measure of the extension of the trap.

In the sequel we shall be considering a limit where a/L_{osc} tends to zero while $N \to \infty$. Experimentally a/L_{osc} can be changed in two ways: One can either vary L_{osc} or a. The first alternative is usually simpler in practice but very recently a direct tuning of the scattering length itself has also been shown to be feasible [13]. Mathematically, both alternatives are equivalent, of course. The first corresponds to writing $V(\mathbf{x}) = L_{\mathrm{osc}}^{-2} V_1(\mathbf{x}/L_{\mathrm{osc}})$ and keeping V_1 and v fixed. The second corresponds to writing the interaction potential as $v(|\mathbf{x}|) = a^{-2} v_1(|\mathbf{x}|/a)$ like in (5.4), where v_1 has unit scattering length, and keeping V and v_1 fixed. This is equivalent to the first, since for given V_1 and v_1 the ground state energy of (6.1), measured in units of $\hbar\omega$, depends only on N and a/L_{osc}. In the dilute limit when a is much smaller than the mean particle distance, the energy becomes independent of v_1.

We choose $L_{\rm osc}$ as a length unit. The energy unit is $\hbar\omega = 2\mu L_{\rm osc}^{-2} = 2\mu$. Moreover, we find it convenient to regard V and v_1 as fixed. This justifies the notion $E_0(N,a)$ for the quantum mechanical ground state energy.

The idea is now to use the information about the thermodynamic limiting energy of the dilute Bose gas in a box to find the ground state energy of (6.1) in an appropriate limit. This has been done in [53, 54] and in this section we give an account of this work. As we saw in Sects. 2 and 3 there is a difference in the ρ dependence between two and three dimensions, so we can expect a related difference now. We discuss 3D first.

6.1 Three Dimensions

Associated with the quantum mechanical ground state energy problem is the Gross–Pitaevskii (GP) energy functional [30, 31, 71]

$$\mathcal{E}^{\rm GP}[\phi] = \int_{\mathbb{R}^3} \left(\mu|\nabla\phi|^2 + V|\phi|^2 + 4\pi\mu a|\phi|^4\right) \mathrm{d}\mathbf{x} \tag{6.2}$$

with the subsidiary condition

$$\int_{\mathbb{R}^3} |\phi|^2 = N\ . \tag{6.3}$$

As before, $a > 0$ is the scattering length of v. The corresponding energy is

$$E^{\rm GP}(N,a) = \inf_{\int|\phi|^2=N} \mathcal{E}^{\rm GP}[\phi] = \mathcal{E}^{\rm GP}[\phi^{\rm GP}]\ , \tag{6.4}$$

with a unique, positive $\phi^{\rm GP}$. The existence of the minimizer $\phi^{\rm GP}$ is proved by standard techniques and it can be shown to be continuously differentiable, see [53], Sect. 2 and Appendix A. The minimizer depends on N and a, of course, and when this is important we denote it by $\phi^{\rm GP}_{N,a}$.

The variational equation satisfied by the minimizer is the *GP equation*

$$-\mu\Delta\phi^{\rm GP}(\mathbf{x}) + V(\mathbf{x})\phi^{\rm GP}(\mathbf{x}) + 8\pi\mu a\phi^{\rm GP}(\mathbf{x})^3 = \mu^{\rm GP}\phi^{\rm GP}(\mathbf{x})\ , \tag{6.5}$$

where $\mu^{\rm GP}$ is the chemical potential, given by

$$\mu^{\rm GP} = \mathrm{d}E^{\rm GP}(N,a)/\mathrm{d}N = E^{\rm GP}(N,a)/N + (4\pi\mu a/N)\int|\phi^{\rm GP}(\mathbf{x})|^4\mathrm{d}\mathbf{x}\ . \tag{6.6}$$

The GP theory has the following scaling property:

$$E^{\rm GP}(N,a) = NE^{\rm GP}(1,Na)\ , \tag{6.7}$$

and

$$\phi^{\rm GP}_{N,a}(\mathbf{x}) = N^{1/2}\phi^{\rm GP}_{1,Na}(\mathbf{x})\ . \tag{6.8}$$

Hence we see that the relevant parameter in GP theory is the combination Na.

We now turn to the relation of E^{GP} and ϕ^{GP} to the quantum mechanical ground state. If $v = 0$, then the ground state of (6.1) is

$$\Psi_0(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \prod_{i=1}^{N} \phi_0(\mathbf{x}_i) \tag{6.9}$$

with ϕ_0 the normalized ground state of $-\mu\Delta + V(\mathbf{x})$. In this case clearly $\phi^{\mathrm{GP}} = \sqrt{N}\ \phi_0$, and then $E^{\mathrm{GP}} = N\hbar\omega = E_0$. In the other extreme, if $V(\mathbf{x}) = 0$ for $\mathbf{x}$ inside a large box of volume L^3 and $V(\mathbf{x}) = \infty$ otherwise, then $\phi^{\mathrm{GP}} \approx \sqrt{N/L^3}$ and we get $E^{\mathrm{GP}}(N, a) = 4\pi\mu a N^2/L^3$, which is the previously considered energy E_0 for the homogeneous gas in the low density regime. (In this case, the gradient term in $\mathcal{E}^{\mathrm{GP}}$ plays no role.)

In general, we expect that for *dilute* gases in a suitable limit

$$E_0 \approx E^{\mathrm{GP}} \quad \text{and} \quad \rho^{\mathrm{QM}}(\mathbf{x}) \approx \left|\phi^{\mathrm{GP}}(\mathbf{x})\right|^2 \equiv \rho^{\mathrm{GP}}(\mathbf{x}) \ , \tag{6.10}$$

where the quantum mechanical particle density in the ground state is defined by

$$\rho^{\mathrm{QM}}(\mathbf{x}) = N \int |\Psi_0(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)|^2 \mathrm{d}\mathbf{x}_2 \cdots \mathrm{d}\mathbf{x}_N \ . \tag{6.11}$$

Dilute means here that

$$\bar{\rho} a^3 \ll 1 \ , \tag{6.12}$$

where

$$\bar{\rho} = \frac{1}{N} \int |\rho^{\mathrm{GP}}(\mathbf{x})|^2 \mathrm{d}\mathbf{x} \tag{6.13}$$

is the *mean density.*

The limit in which (6.10) can be expected to be true should be chosen so that *all three* terms in $\mathcal{E}^{\mathrm{GP}}$ make a contribution. The scaling relations (6.7) and (6.8) indicate that fixing Na as $N \to \infty$ is the right thing to do (and this is quite relevant since experimentally N can be quite large, 10^6 and more, and Na can range from about 1 to 10^4 [14]). Fixing Na (which we refer to as the GP case) also means that we really are dealing with a dilute limit, because the mean density $\bar{\rho}$ is then of the order N (since $\bar{\rho}_{N,a} = N\bar{\rho}_{1,Na}$) and hence

$$a^3 \bar{\rho} \sim N^{-2} \ . \tag{6.14}$$

The precise statement of (6.10) is:

Theorem 6.1 (GP limit of the QM ground state energy and density). *If $N \to \infty$ with Na fixed, then*

$$\lim_{N\to\infty} \frac{E_0(N, a)}{E^{\mathrm{GP}}(N, a)} = 1 \ , \tag{6.15}$$

and

$$\lim_{N\to\infty} \frac{1}{N} \rho^{\mathrm{QM}}_{N,a}(\mathbf{x}) = \left|\phi^{\mathrm{GP}}_{1,Na}(\mathbf{x})\right|^2 \tag{6.16}$$

in the weak L^1-sense.

Convergence can not only be proved for the ground state energy and density, but also for the individual energy components:

Theorem 6.2 (Asymptotics of the energy components). *Let ψ_0 denote the solution to the zero-energy scattering equation for v (under the boundary condition $\lim_{|\mathbf{x}|\to\infty}\psi_0(\mathbf{x})=1$) and $s=\int|\nabla\psi_0|^2/(4\pi a)$. Then $0<s\leq 1$ and, in the same limit as in Theorem 6.1 above,*

$$\lim_{N\to\infty}\int|\nabla_{\mathbf{x}_1}\Psi_0(\mathbf{x}_1,\mathbf{X})|^2\mathrm{d}\mathbf{x}_1\,\mathrm{d}\mathbf{X} = \int|\nabla\phi^{\mathrm{GP}}_{1,Na}(\mathbf{x})|^2\mathrm{d}\mathbf{x}+4\pi Nas\int|\phi^{\mathrm{GP}}_{1,Na}(\mathbf{x})|^4\mathrm{d}\mathbf{x}\,, \tag{6.17a}$$

$$\lim_{N\to\infty}\int V(\mathbf{x}_1)|\Psi_0(\mathbf{x}_1,\mathbf{X})|^2\mathrm{d}\mathbf{x}_1\,\mathrm{d}\mathbf{X}=\int V(\mathbf{x})|\phi^{\mathrm{GP}}_{1,Na}(\mathbf{x})|^2\mathrm{d}\mathbf{x}\,, \tag{6.17b}$$

$$\lim_{N\to\infty}\tfrac12\sum_{j=2}^{N}\int v(|\mathbf{x}_1-\mathbf{x}_j|)|\Psi_0(\mathbf{x}_1,\mathbf{X})|^2\mathrm{d}\mathbf{x}_1\,\mathrm{d}\mathbf{X} = (1-s)4\pi Na\int|\phi^{\mathrm{GP}}_{1,Na}(\mathbf{x})|^4\mathrm{d}\mathbf{x}\,. \tag{6.17c}$$

Here we introduced again the short hand notation (5.2). Theorem 6.2 is a simple consequence of Theorem 6.1 by variation with respect to the different components of the energy, as was also noted in [11]. More precisely, (6.15) can be written as

$$\lim_{N\to\infty}\frac{1}{N}E_0(N,a)=E^{\mathrm{GP}}(1,Na)\,. \tag{6.18}$$

The ground state energy is a concave function of the mass parameter μ, so it is legitimate to differentiate both sides of (6.18) with respect to μ. In doing so, it has to be noted that Na depends on μ through the scattering length. Using (2.13) one sees that

$$\frac{\mathrm{d}(\mu a)}{\mathrm{d}\mu}=\frac{1}{4\pi}\int|\nabla\psi_0|^2\mathrm{d}\mathbf{x} \tag{6.19}$$

by the Feynman–Hellmann principle, since ψ_0 minimizes the left side of (2.13).

We remark that in the case of a two-dimensional Bose gas, where the relevant parameter to be kept fixed in the GP limit is $N/|\ln(a^2\bar\rho_N)|$ (c.f. Sects. 3 and 6.2.), the parameter s in Theorem 6.2 can be shown to be always equal to 1. I.e., in 2D the interaction energy is purely kinetic in the GP limit (see [10]).

To describe situations where Na is very large, it is appropriate to consider a limit where, as $N\to\infty$, $a\gg N^{-1}$, i.e. $Na\to\infty$, but still $\bar\rho a^3\to 0$. In this case, the gradient term in the GP functional becomes negligible compared to the other terms and the so-called *Thomas–Fermi (TF) functional*

$$\mathcal{E}^{\mathrm{TF}}[\rho] = \int_{\mathbb{R}^3} \left(V\rho + 4\pi\mu a\rho^2\right) \mathrm{d}\mathbf{x} \tag{6.20}$$

arises. (Note that this functional has nothing to do with the fermionic theory invented by Thomas and Fermi in 1927, except for a certain formal analogy.) It is defined for nonnegative functions ρ on $\mathbb{R}^3$. Its ground state energy E^{TF} and density ρ^{TF} are defined analogously to the GP case. (The TF functional is especially relevant for the two-dimensional Bose gas. There a has to decrease exponentially with N in the GP limit, so the TF limit is more adequate; see Sect. 6.2 below).

Our second main result of this section is that minimization of (6.20) reproduces correctly the ground state energy and density of the many-body Hamiltonian in the limit when $N \to \infty$, $a^3\bar{\rho} \to 0$, but $Na \to \infty$ (which we refer to as the TF case), provided the external potential is reasonably well behaved. We will assume that V is asymptotically equal to some function W that is homogeneous of some order $s > 0$, i.e., $W(\lambda\mathbf{x}) = \lambda^s W(\mathbf{x})$ for all $\lambda > 0$, and locally Hölder continuous (see [54] for a precise definition). This condition can be relaxed, but it seems adequate for most practical applications and simplifies things considerably.

Theorem 6.3 (TF limit of the QM ground state energy and density). *Assume that V satisfies the conditions stated above. If $g \equiv Na \to \infty$ as $N \to \infty$, but still $a^3\bar{\rho} \to 0$, then*

$$\lim_{N\to\infty} \frac{E_0(N,a)}{E^{\mathrm{TF}}(N,a)} = 1\ , \tag{6.21}$$

and

$$\lim_{N\to\infty} \frac{g^{3/(s+3)}}{N} \rho^{\mathrm{QM}}_{N,a}(g^{1/(s+3)}\mathbf{x}) = \tilde{\rho}^{\mathrm{TF}}_{1,1}(\mathbf{x}) \tag{6.22}$$

in the weak L^1-sense, where $\tilde{\rho}^{\mathrm{TF}}_{1,1}$ is the minimizer of the TF functional under the condition $\int \rho = 1$, $a = 1$, and with V replaced by W.

In the following, we will present the essentials of the proofs Theorems 6.1 and 6.3. We will derive appropriate upper and lower bounds on the ground state energy E_0.

The proof of the lower bound in Theorem 6.1 presented here is a modified version of (and partly simpler than) the original proof in [53].

The convergence of the densities follows from the convergence of the energies in the usual way by variation with respect to the external potential. For simplicity, we set $\mu \equiv 1$ in the following.

Proof (Theorems 6.1 and 6.3). Part 1: Upper bound to the QM energy. To derive an upper bound on E_0 we use a generalization of a trial wave function of Dyson [17], who used this function to give an upper bound on the ground state energy of the homogeneous hard core Bose gas (c.f. Sect. 2.1). It is of the form

$$\Psi(\mathbf{x}_1,\dots,\mathbf{x}_N) = \prod_{i=1}^N \phi^{\mathrm{GP}}(\mathbf{x}_i)F(\mathbf{x}_1,\dots,\mathbf{x}_N)\ , \tag{6.23}$$

where F is constructed in the following way:

$$F(\mathbf{x}_1,\dots,\mathbf{x}_N) = \prod_{i=1}^N f(t_i(\mathbf{x}_1,\dots,\mathbf{x}_i))\ , \tag{6.24}$$

where $t_i = \min\{|\mathbf{x}_i - \mathbf{x}_j|, 1 \le j \le i-1\}$ is the distance of $\mathbf{x}_i$ to its *nearest neighbor* among the points $\mathbf{x}_1,\dots,\mathbf{x}_{i-1}$, and f is a function of $r \ge 0$. As in (2.20) we choose it to be

$$f(r) = \begin{cases} f_0(r)/f_0(b) & \text{for} \quad r < b\ , \\ 1 & \text{for} \quad r \ge b\ , \end{cases} \tag{6.25}$$

where f_0 is the solution of the zero energy scattering equation (2.3) and b is some cut-off parameter of order $b \sim \bar\rho^{-1/3}$. The function (6.23) is not totally symmetric, but for an upper bound it is nevertheless an acceptable test wave function since the bosonic ground state energy is equal to the *absolute* ground state energy.

The result of a somewhat lengthy computation (see [53] for details) is the upper bound

$$E_0(N,a) \le E^{\mathrm{GP}}(N,a)\left(1 + O(a\bar\rho^{1/3})\right)\ . \tag{6.26}$$

Part 2: Lower bound to the QM energy, GP case. To obtain a lower bound for the QM ground state energy the strategy is to divide space into boxes and use the estimate on the homogeneous gas, given in Theorem 2.4, in each box with *Neumann* boundary conditions. One then minimizes over all possible divisions of the particles among the different boxes. This gives a lower bound to the energy because discontinuous wave functions for the quadratic form defined by the Hamiltonian are now allowed. We can neglect interactions among particles in different boxes because $v \ge 0$. Finally, one lets the box size tend to zero. However, it is not possible to simply approximate V by a constant potential in each box. To see this consider the case of noninteracting particles, i.e., $v = 0$ and hence $a = 0$. Here $E_0 = N\hbar\omega$, but a 'naive' box method gives only $\min_{\mathbf{x}} V(\mathbf{x})$ as lower bound, since it clearly pays to put all the particles with a constant wave function in the box with the lowest value of V.

For this reason we start by separating out the GP wave function in each variable and write a general wave function Ψ as

$$\Psi(\mathbf{x}_1,\dots,\mathbf{x}_N) = \prod_{i=1}^N \phi^{\mathrm{GP}}(\mathbf{x}_i)F(\mathbf{x}_1,\dots,\mathbf{x}_N)\ . \tag{6.27}$$

Here $\phi^{\mathrm{GP}} = \phi^{\mathrm{GP}}_{N,a}$ is normalized so that $\int |\phi^{\mathrm{GP}}|^2 = N$. Equation (6.27) defines F for a given Ψ because ϕ^{GP} is everywhere strictly positive, being the ground state of the operator $-\Delta + V + 8\pi a|\phi^{\rm GP}|^2$. We now compute the expectation value of H in the state Ψ. Using partial integration and the variational equation (6.5) for $\phi^{\rm GP}$, we see that

$$\frac{\langle \Psi | H\Psi\rangle}{\langle \Psi|\Psi\rangle} - E^{\rm GP}(N,a) = 4\pi a \int |\rho^{\rm GP}|^2 + Q(F)\ , \tag{6.28}$$

with

$$Q(F) = \sum_{i=1}^N \frac{\int \prod_{k=1}^N \rho^{\rm GP}(\mathbf{x}_k) \left(|\nabla_i F|^2 + \left[\frac{1}{2}\sum_{j\neq i} v(|\mathbf{x}_i - \mathbf{x}_j|) - 8\pi a \rho^{\rm GP}(\mathbf{x}_i)\right] |F|^2\right)}{\int \prod_{k=1}^N \rho^{\rm GP}(\mathbf{x}_k)|F|^2}\ . \tag{6.29}$$

We recall that $\rho^{\rm GP}(\mathbf{x}) = |\phi^{\rm GP}_{N,a}(\mathbf{x})|^2$. For computing the ground state energy of H we have to minimize the normalized quadratic form Q. Compared to the expression for the energy involving Ψ itself we have thus obtained the replacements

$$V(\mathbf{x}) \to -8\pi a \rho^{\rm GP}(\mathbf{x}) \quad \text{and} \quad \prod_{i=1}^N d\mathbf{x}_i \to \prod_{i=1}^N \rho^{\rm GP}(\mathbf{x}_i) \mathrm{d}\mathbf{x}_i\ . \tag{6.30}$$

We now use the box method on *this* problem. More precisely, labeling the boxes by an index α, we have

$$\inf_F Q(F) \geq \inf_{\{n_\alpha\}} \sum_\alpha \inf_{F_\alpha} Q_\alpha(F_\alpha)\ , \tag{6.31}$$

where Q_α is defined by the same formula as Q but with the integrations limited to the box α, F_α is a wave function with particle number n_α, and the infimum is taken over all distributions of the particles with $\sum n_\alpha = N$.

We now fix some $M > 0$, that will eventually tend to ∞, and restrict ourselves to boxes inside a cube Λ_M of side length M. Since $v \geq 0$ the contribution to (6.31) of boxes outside this cube is easily estimated from below by $-8\pi N a \sup_{\mathbf{x}\notin\Lambda_M} \rho^{\rm GP}(\mathbf{x})$, which, divided by N, is arbitrarily small for M large, since Na is fixed and $\phi^{\rm GP}/N^{1/2} = \phi^{\rm GP}_{1,Na}$ decreases faster than exponentially at infinity ([53], Lemma A.5).

For the boxes inside the cube Λ_M we want to use Lemma 2.5 and therefore we must approximate $\rho^{\rm GP}$ by constants in each box. Let $\rho_{\alpha,\max}$ and $\rho_{\alpha,\min}$, respectively, denote the maximal and minimal values of $\rho^{\rm GP}$ in box α. Define

$$\Psi_\alpha(\mathbf{x}_1,\dots,\mathbf{x}_{n_\alpha}) = F_\alpha(\mathbf{x}_1,\dots,\mathbf{x}_{n_\alpha}) \prod_{k=1}^{n_\alpha} \phi^{\rm GP}(\mathbf{x}_k)\ , \tag{6.32}$$

and

$$\Psi_\alpha^{(i)}(\mathbf{x}_1,\ldots,\mathbf{x}_{n_\alpha}) = F_\alpha(\mathbf{x}_1,\ldots,\mathbf{x}_{n_\alpha}) \prod_{\substack{k=1\\k\neq i}}^{n_\alpha} \phi^{\rm GP}(\mathbf{x}_k)\ . \tag{6.33}$$

We have, for all $1 \leq i \leq n_\alpha$,

$$\begin{aligned} \int \prod_{k=1}^{n_\alpha} \rho^{\rm GP}(\mathbf{x}_k) \left(|\nabla_i F_\alpha|^2 + \tfrac{1}{2}\sum_{j\neq i} v(|\mathbf{x}_i-\mathbf{x}_j|)|F_\alpha|^2\right) \\ \geq \rho_{\alpha,\min} \int \left(|\nabla_i \Psi_\alpha^{(i)}|^2 + \tfrac{1}{2}\sum_{j\neq i} v(|\mathbf{x}_i-\mathbf{x}_j|)|\Psi_\alpha^{(i)}|^2\right)\ . \end{aligned} \tag{6.34}$$

We now use Lemma 2.5 to get, for all $0 \leq \varepsilon \leq 1$,

$$(6.34) \geq \rho_{\alpha,\min} \int \left(\varepsilon|\nabla_i \Psi_\alpha^{(i)}|^2 + a(1-\varepsilon)U(t_i)|\Psi_\alpha^{(i)}|^2\right) \tag{6.35}$$

where t_i is the distance to the nearest neighbor of $\mathbf{x}_i$, c.f., (2.29), and U the potential (2.30).

Since $\Psi_\alpha = \phi^{\rm GP}(\mathbf{x}_i)\Psi_\alpha^{(i)}$ we can estimate

$$|\nabla_i \Psi_\alpha|^2 \leq 2\rho_{\alpha,\max}|\nabla_i \Psi_\alpha^{(i)}|^2 + 2|\Psi_\alpha^{(i)}|^2 N C_M \tag{6.36}$$

with

$$C_M = \frac{1}{N}\sup_{\mathbf{x}\in\Lambda_M} |\nabla\phi^{\rm GP}(\mathbf{x})|^2 = \sup_{\mathbf{x}\in\Lambda_M} |\nabla\phi^{\rm GP}_{1,Na}(\mathbf{x})|^2\ . \tag{6.37}$$

Since Na is fixed, C_M is independent of N. Inserting (6.36) into (6.35), summing over i and using $\rho^{\rm GP}(\mathbf{x}_i) \leq \rho_{\alpha,\max}$ in the last term of (6.29) (in the box α), we get

$$Q_\alpha(F_\alpha) \geq \frac{\rho_{\alpha,\min}}{\rho_{\alpha,\max}} E^U_\varepsilon(n_\alpha, L) - 8\pi a\rho_{\alpha,\max} n_\alpha - \varepsilon C_M n_\alpha\ , \tag{6.38}$$

where L is the side length of the box and $E^U_\varepsilon(n_\alpha,L)$ is the ground state energy of

$$\sum_{i=1}^{n_\alpha}(-\tfrac{1}{2}\varepsilon\Delta_i + (1-\varepsilon)aU(t_i)) \tag{6.39}$$

in the box (c.f. (2.35)). We want to minimize (6.38) with respect to n_α and drop the subsidiary condition $\sum_\alpha n_\alpha = N$ in (6.31). This can only lower the minimum. For the time being we also ignore the last term in (6.38). (The total contribution of this term for all boxes is bounded by $\varepsilon C_M N$ and will be shown to be negligible compared to the other terms.)

Since the lower bound for the energy of Theorem 2.4 was obtained precisely from a lower bound to the operator (6.39), we can use the statement and proof of Theorem 2.4. From this we see that

$$E^U_\varepsilon(n_\alpha, L) \geq (1-\varepsilon)\frac{4\pi a n_\alpha^2}{L^3}(1 - CY_\alpha^{1/17}) \tag{6.40}$$

with $Y_\alpha = a^3 n_\alpha / L^3$, provided Y_α is small enough, $\varepsilon \geq Y_\alpha^{1/17}$ and $n_\alpha \geq (\text{const.}) Y_\alpha^{-1/17}$. The condition on ε is certainly fulfilled if we choose $\varepsilon = Y^{1/17}$ with $Y = a^3 N/L^3$. We now want to show that the n_α minimizing the right side of (6.38) is large enough for (6.40) to apply.

If the minimum of the right side of (6.38) (without the last term) is taken for some $\bar{n}_\alpha$, we have

$$\frac{\rho_{\alpha,\min}}{\rho_{\alpha,\max}} \left(E_\varepsilon^U(\bar{n}_\alpha + 1, L) - E_\varepsilon^U(\bar{n}_\alpha, L) \right) \geq 8\pi a \rho_{\alpha,\max} \,. \tag{6.41}$$

On the other hand, we claim that

Lemma 6.4. *For any n*

$$E_\varepsilon^U(n+1, L) - E_\varepsilon^U(n, L) \leq 8\pi a \frac{n}{L^3} \,. \tag{6.42}$$

Proof. Denote the operator (6.39) by $\tilde{H}_n$, with $n_\alpha = n$, and let $\tilde{\Psi}_n$ be its ground state. Let t_i' be the distance to the nearest neighbor of $\mathbf{x}_i$ among the $n+1$ points $\mathbf{x}_1, \ldots, \mathbf{x}_{n+1}$ (without $\mathbf{x}_i$) and t_i the corresponding distance excluding $\mathbf{x}_{n+1}$. Obviously, for $1 \leq i \leq n$,

$$U(t_i') \leq U(t_i) + U(|\mathbf{x}_i - \mathbf{x}_{n+1}|) \tag{6.43}$$

and

$$U(t_{n+1}') \leq \sum_{i=1}^{n} U(|\mathbf{x}_i - \mathbf{x}_{n+1}|) \,. \tag{6.44}$$

Therefore

$$\tilde{H}_{n+1} \leq \tilde{H}_n - \tfrac{1}{2}\varepsilon \Delta_{n+1} + 2a \sum_{i=1}^{n} U(|\mathbf{x}_i - \mathbf{x}_{n+1}|) \,. \tag{6.45}$$

Using $\tilde{\Psi}_n / L^{3/2}$ as trial function for $\tilde{H}_{n+1}$ we arrive at (6.42). □

Equation (6.42) together with (6.41) shows that $\bar{n}_\alpha$ is at least $\sim \rho_{\alpha,\max} L^3$. We shall choose $L \sim N^{-1/10}$, so the conditions needed for (6.40) are fulfilled for N large enough, since $\rho_{\alpha,\max} \sim N$ and hence $\bar{n}_\alpha \sim N^{7/10}$ and $Y_\alpha \sim N^{-2}$.

In order to obtain a lower bound on Q_α we therefore have to minimize

$$4\pi a \left(\frac{\rho_{\alpha,\min}}{\rho_{\alpha,\max}} \frac{n_\alpha^2}{L^3} \left(1 - C Y^{1/17}\right) - 2 n_\alpha \rho_{\alpha,\max} \right) \,. \tag{6.46}$$

We can drop the requirement that n_α has to be an integer. The minimum of (6.46) is obtained for

$$n_\alpha = \frac{\rho_{\alpha,\max}^2}{\rho_{\alpha,\min}} \frac{L^3}{(1 - C Y^{1/17})} \,. \tag{6.47}$$

By (6.28) this gives the following lower bound, including now the last term in (6.38) as well as the contributions from the boxes outside Λ_M,

$$
\begin{aligned}
&E_0(N,a) - E^{\mathrm{GP}}(N,a) \\
&\qquad \geq 4\pi a \int |\rho^{\mathrm{GP}}|^2 - 4\pi a \sum_{\alpha \subset \Lambda_M} \rho_{\alpha,\min}^2 L^3 \left(\frac{\rho_{\alpha,\max}^3}{\rho_{\alpha,\min}^3} \frac{1}{(1 - CY^{1/17})} \right) \\
&\qquad\quad - Y^{1/17} N C_M - 4\pi a N \sup_{\mathbf{x} \notin \Lambda_M} \rho^{\mathrm{GP}}(\mathbf{x}) \ .
\end{aligned} \tag{6.48}
$$

Now ρ^{GP} is differentiable and strictly positive. Since all the boxes are in the fixed cube Λ_M there are constants $C' < \infty$, $C'' > 0$, such that

$$
\rho_{\alpha,\max} - \rho_{\alpha,\min} \leq NC'L, \quad \rho_{\alpha,\min} \geq NC'' \ . \tag{6.49}
$$

Since $L \sim N^{-1/10}$ and $Y \sim N^{-17/10}$ we therefore have, for large N,

$$
\frac{\rho_{\alpha,\max}^3}{\rho_{\alpha,\min}^3} \frac{1}{(1 - CY^{1/17})} \leq 1 + (\text{const.}) N^{-1/10} \tag{6.50}
$$

Also,

$$
4\pi a \sum_{\alpha \subset \Lambda_M} \rho_{\alpha,\min}^2 L^3 \leq 4\pi a \int |\rho^{\mathrm{GP}}|^2 \leq E^{\mathrm{GP}}(N,a) \ . \tag{6.51}
$$

Hence, noting that $E^{\mathrm{GP}}(N,a) = NE^{\mathrm{GP}}(1,Na) \sim N$ since Na is fixed,

$$
\frac{E_0(N,a)}{E^{\mathrm{GP}}(N,a)} \geq 1 - (\text{const.})(1 + C_M) N^{-1/10} - (\text{const.}) \sup_{\mathbf{x} \notin \Lambda_M} |\phi_{1,Na}^{\mathrm{GP}}|^2 \ , \tag{6.52}
$$

where the constants depend on Na. We can now take $N \to \infty$ and then $M \to \infty$.

Part 3: Lower bound to the QM energy, TF case. In the above proof of the lower bound in the GP case we did not attempt to keep track of the dependence of the constants on Na. In the TF case $Na \to \infty$, so one would need to take a closer look at this dependence if one wanted to carry the proof directly over to this case. But we don't have to do so, because there is a simpler direct proof. Using the explicit form of the TF minimizer, namely

$$
\rho_{N,a}^{\mathrm{TF}}(\mathbf{x}) = \frac{1}{8\pi a} [\mu^{\mathrm{TF}} - V(\mathbf{x})]_+ \ , \tag{6.53}
$$

where $[t]_+ \equiv \max\{t, 0\}$ and μ^{TF} is chosen so that the normalization condition $\int \rho_{N,a}^{\mathrm{TF}} = N$ holds, we can use

$$
V(\mathbf{x}) \geq \mu^{\mathrm{TF}} - 8\pi a \rho^{\mathrm{TF}}(\mathbf{x}) \tag{6.54}
$$

to get a replacement as in (6.30), but without changing the measure. Moreover, ρ^{TF} has compact support, so, applying again the box method described above, the boxes far out do not contribute to the energy. However, μ^{TF} (which depends only on the combination Na) tends to infinity as $Na \to \infty$. We need to control the asymptotic behavior of $\mu^{\rm TF}$, and this leads to the restrictions on V described in the paragraph preceding Theorem 6.3. For simplicity, we shall here only consider the case when V itself is homogeneous, i.e., $V(\lambda\mathbf{x}) = \lambda^s V(\mathbf{x})$ for all $\lambda > 0$ with some $s > 0$.

In the same way as in (6.6) we have, with $g = Na$,

$$\mu^{\rm TF}(g) = {\rm d}E^{\rm TF}(N,a)/{\rm d}N = E^{\rm TF}(1,g) + 4\pi g \int |\rho^{\rm TF}_{1,g}(\mathbf{x})|^2 {\rm d}\mathbf{x} \, . \tag{6.55}$$

The TF energy, chemical potential and minimizer satisfy the scaling relations

$$E^{\rm TF}(1,g) = g^{s/(s+3)} E^{\rm TF}(1,1) \, , \tag{6.56}$$

$$\mu^{\rm TF}(g) = g^{s/(s+3)} \mu^{\rm TF}(1) \, , \tag{6.57}$$

and

$$g^{3/(s+3)} \rho^{\rm TF}_{1,g}(g^{1/(s+3)}\mathbf{x}) = \rho^{\rm TF}_{1,g}(\mathbf{x}) \, . \tag{6.58}$$

We also introduce the scaled interaction potential, $\widehat{v}$, by

$$\widehat{v}(\mathbf{x}) = g^{2/(s+3)} v(g^{1/(s+3)}\mathbf{x}) \tag{6.59}$$

with scattering length

$$\widehat{a} = g^{-1/(s+3)} a \, . \tag{6.60}$$

Using (6.54), (6.55) and the scaling relations we obtain

$$E_0(N,a) \geq E^{\rm TF}(N,a) + 4\pi N g^{s/(s+3)} \int |\rho^{\rm TF}_{1,1}|^2 + g^{-2/(s+3)} Q \tag{6.61}$$

with

$$Q = \inf_{\int |\Psi|^2 = 1} \sum_i \int \Big(|\nabla_i \Psi|^2 + \tfrac{1}{2} \sum_{j \neq i} \widehat{v}(\mathbf{x}_i - \mathbf{x}_j)|\Psi|^2 - 8\pi N \widehat{a} \rho^{\rm TF}_{1,1}(\mathbf{x}_i)|\Psi|^2 \Big) \, . \tag{6.62}$$

We can now proceed exactly as in Part 2 to arrive at the analogy of (6.48), which in the present case becomes

$$\begin{aligned} E_0(N,a) - E^{\rm TF}(N,a) \geq 4\pi N g^{s/(s+3)} & \int |\rho^{\rm TF}_{1,1}|^2 \\ & - 4\pi N \widehat{a} \sum_\alpha \rho^2_{\alpha,\max} L^3 (1 - C\widehat{Y}^{1/17})^{-1} \, . \end{aligned} \tag{6.63}$$

Here $\rho_{\alpha,\max}$ is the maximum of $\rho^{\rm TF}_{1,1}$ in the box α, and $\widehat{Y} = \widehat{a}^3 N/L^3$. This holds as long as L does not decrease too fast with N. In particular, if L is simply fixed, this holds for all large enough N. Note that

$$\bar{\rho} = N \bar{\rho}_{1,g} \sim N g^{-3/(s+3)} \bar{\rho}_{1,1} \, , \tag{6.64}$$

so that $\widehat{a}^3 N \sim a^3\bar{\rho}$ goes to zero as $N \to \infty$ by assumption. Hence, if we first let $N \to \infty$ (which implies $\widehat{Y} \to 0$) and then take L to zero, we of arrive at the desired result

$$\liminf_{N\to\infty} \frac{E_0(N,a)}{E^{\rm TF}(N,a)} \geq 1 \tag{6.65}$$

in the limit $N \to \infty$, $a^3\bar{\rho} \to 0$. Here we used the fact that (because V, and hence $\rho^{\rm TF}$, is continuous by assumption) the Riemann sum $\sum_\alpha \rho_{\alpha,\max}^2 L^3$ converges to $\int |\rho_{1,1}^{\rm TF}|^2$ as $L \to 0$. Together with the upper bound (6.26) and the fact that $E^{\rm GP}(N,a)/E^{\rm TF}(N,a) = E^{\rm GP}(1,Na)/E^{\rm TF}(1,Na) \to 1$ as $Na \to \infty$, which holds under our regularity assumption on V (c.f. Lemma 2.3 in [54]), this proves (6.15) and (6.21).

Part 4: Convergence of the densities. The convergence of the energies implies the convergence of the densities in the usual way by variation of the external potential. We show here the TF case, the GP case goes analogously. Set again $g = Na$. Making the replacement

$$V(\mathbf{x}) \longrightarrow V(\mathbf{x}) + \delta g^{s/(s+3)} Z(g^{-1/(s+3)}\mathbf{x}) \tag{6.66}$$

for some positive $Z \in C_0^\infty$ and redoing the upper and lower bounds we see that (6.21) holds with W replaced by $W + \delta Z$. Differentiating with respect to δ at $\delta = 0$ yields

$$\lim_{N\to\infty} \frac{g^{3/(s+3)}}{N} \rho_{N,a}^{\rm QM}(g^{1/(s+3)}\mathbf{x}) = \tilde{\rho}_{1,1}^{\rm TF}(\mathbf{x}) \tag{6.67}$$

in the sense of distributions. Since the functions all have L^1-norm 1, we can conclude that there is even weak L^1-convergence. □

6.2 Two Dimensions

In contrast to the three-dimensional case the energy per particle for a dilute gas in two dimensions is *nonlinear* in ρ. In view of Schick's formula (3.1) for the energy of the homogeneous gas it would appear natural to take the interaction into account in two dimensional GP theory by a term

$$4\pi \int_{\mathbb{R}^2} |\ln(|\phi(\mathbf{x})|^2 a^2)|^{-1} |\phi(\mathbf{x})|^4 d\mathbf{x} \,, \tag{6.68}$$

and such a term has, indeed, been suggested in [80] and [40]. However, since the nonlinearity appears only in a logarithm, this term is unnecessarily complicated as far as leading order computations are concerned. For dilute gases it turns out to be sufficient, to leading order, to use an interaction term of the same form as in the three-dimensional case, i.e, define the GP functional as (for simplicity we put $\mu = 1$ in this section)

$$\mathcal{E}^{\mathrm{GP}}[\phi] = \int_{\mathbb{R}^2} \left(|\nabla\phi|^2 + V|\phi|^2 + 4\pi\alpha|\phi|^4 \right) \mathrm{d}\mathbf{x} \,, \tag{6.69}$$

where instead of a the coupling constant is now

$$\alpha = |\ln(\bar{\rho}_N a^2)|^{-1} \tag{6.70}$$

with $\bar{\rho}_N$ the *mean density* for the GP functional at coupling constant 1 and particle number N. This is defined analogously to (6.13) as

$$\bar{\rho}_N = \frac{1}{N} \int |\phi^{\mathrm{GP}}_{N,1}|^4 \mathrm{d}\mathbf{x} \tag{6.71}$$

where $\phi^{\mathrm{GP}}_{N,1}$ is the minimizer of (6.69) with $\alpha = 1$ and subsidiary condition $\int |\phi|^2 = N$. Note that α in (6.70) depends on N through the mean density.

Let us denote the GP energy for a given N and coupling constant α by $E^{\mathrm{GP}}(N,\alpha)$ and the corresponding minimizer by $\phi^{\mathrm{GP}}_{N,\alpha}$. As in three dimensions the scaling relations

$$E^{\mathrm{GP}}(N,\alpha) = N E^{\mathrm{GP}}(1, N\alpha) \tag{6.72}$$

and

$$N^{-1/2}\phi^{\mathrm{GP}}_{N,\alpha} = \phi^{\mathrm{GP}}_{1,N\alpha} \,, \tag{6.73}$$

hold, and the relevant parameter is

$$g \equiv N\alpha \,. \tag{6.74}$$

In three dimensions, where $\alpha = a$, it is natural to consider the limit $N \to \infty$ with $g = Na=$ const. The analogue of Theorem 6.1 in two dimensions is

Theorem 6.5 (Two-dimensional GP limit theorem). *If, for* $N \to \infty$, $a^2\bar{\rho}_N \to 0$ *with* $g = N/|\ln(a^2\bar{\rho}_N)|$ *fixed, then*

$$\lim_{N\to\infty} \frac{E_0(N,a)}{E^{GP}(N, 1/|\ln(a^2\bar{\rho}_N)|)} = 1 \tag{6.75}$$

and

$$\lim_{N\to\infty} \frac{1}{N} \rho^{\mathrm{QM}}_{N,a}(\mathbf{x}) = \left|\phi^{\mathrm{GP}}_{1,g}(\mathbf{x})\right|^2 \tag{6.76}$$

in the weak L^1*-sense.*

This result, however, is of rather limited use in practice. The reason is that in two dimensions the scattering length has to decrease exponentially with N if g is fixed. The parameter g is typically *very large* in two dimensions so it is more appropriate to consider the limit $N \to \infty$ and $g \to \infty$ (but still $\bar{\rho}_N a^2 \to 0$).

For potentials V that are *homogeneous* functions of $\mathbf{x}$, i.e.,

$$V(\lambda \mathbf{x}) = \lambda^s V(\mathbf{x}) \tag{6.77}$$

for some $s > 0$, this limit can be described by the a 'Thomas–Fermi' energy functional like (6.20) with coupling constant unity:

$$\mathcal{E}^{\mathrm{TF}}[\rho] = \int_{\mathbb{R}^2} \left(V(\mathbf{x})\rho(\mathbf{x}) + 4\pi\rho(\mathbf{x})^2\right) \mathrm{d}\mathbf{x} \; . \tag{6.78}$$

This is just the GP functional without the gradient term and $\alpha = 1$. Here ρ is a nonnegative function on $\mathbb{R}^2$ and the normalization condition is

$$\int \rho(\mathbf{x}) \mathrm{d}\mathbf{x} = 1 \; . \tag{6.79}$$

The minimizer of (6.78) can be given explicitly. It is

$$\rho^{\mathrm{TF}}_{1,1}(\mathbf{x}) = (8\pi)^{-1}[\mu^{\mathrm{TF}} - V(\mathbf{x})]_+ \tag{6.80}$$

where the chemical potential μ^{TF} is determined by the normalization condition (6.79) and $[t]_+ = t$ for $t \geq 0$ and zero otherwise. We denote the corresponding energy by $E^{\mathrm{TF}}(1,1)$. By scaling one obtains

$$\lim_{g \to \infty} E^{\mathrm{GP}}(1,g)/g^{s/(s+2)} = E^{\mathrm{TF}}(1,1) \; , \tag{6.81}$$

$$\lim_{g \to \infty} g^{2/(s+2)} \rho^{\mathrm{GP}}_{1,g}(g^{1/(s+2)}\mathbf{x}) = \rho^{\mathrm{TF}}_{1,1}(\mathbf{x}) \; , \tag{6.82}$$

with the latter limit in the strong L^2 sense.

Our main result about two-dimensional Bose gases in external potentials satisfying (6.77) is that analogous limits also hold for the many-particle quantum mechanical ground state at low densities:

Theorem 6.6 (Two-dimensional TF limit theorem). *In two dimensions, if $a^2\bar{\rho}_N \to 0$, but $g = N/|\ln(\bar{\rho}_N a^2)| \to \infty$ as $N \to \infty$ then*

$$\lim_{N \to \infty} \frac{E_0(N,a)}{g^{s/s+2}} = E^{\mathrm{TF}}(1,1) \tag{6.83}$$

and, in the weak L^1 sense,

$$\lim_{N \to \infty} \frac{g^{2/(s+2)}}{N} \rho^{\mathrm{QM}}_{N,a}(g^{1/(s+2)}\mathbf{x}) = \rho^{\mathrm{TF}}_{1,1}(\mathbf{x}) \; . \tag{6.84}$$

Remarks. 1. As in Theorem 6.3, it is sufficient that V is asymptotically equal to some homogeneous potential, W. In this case, $E^{\mathrm{TF}}(1,1)$ and $\rho^{\mathrm{TF}}_{1,1}$ in Theorem 6.6 should be replaced by the corresponding quantities for W.

2. From (6.82) it follows that

$$\bar{\rho}_N \sim N^{s/(s+2)} \tag{6.85}$$

for large N. Hence the low density criterion $a^2\bar{\rho} \ll 1$, means that $a/L_{\mathrm{osc}} \ll N^{-s/2(s+2)}$.

We shall now comment briefly on the proofs of Theorems 6.5 and 6.6, mainly pointing out the differences from the 3D case considered previously.

The upper bounds for the energy are obtained exactly in a same way as in three dimensions. For the lower bound in Theorem 6.5 the point to notice is that the expression (6.46), that has to be minimized over n_α, is in 2D replaced by

$$4\pi\left(\frac{\rho_{\alpha,\min}}{\rho_{\alpha,\max}}\frac{n_\alpha^2}{L^2}\frac{1}{|\ln(a^2n_\alpha/L^2)|}\left(1-\frac{C}{|\ln(a^2N/L^2)|^{1/5}}\right)-\frac{2n_\alpha\rho_{\alpha,\max}}{|\ln(a^2\bar{\rho}_N)|}\right), \tag{6.86}$$

since (6.40) has to be replaced by the analogous inequality for 2D (c.f. (3.31)). To minimize (6.86) we use the following lemma:

Lemma 6.7. *For* $0<x,b<1$ *and* $k\geq 1$ *we have*

$$\frac{x^2}{|\ln x|}-2\frac{b}{|\ln b|}xk\geq -\frac{b^2}{|\ln b|}\left(1+\frac{1}{(2|\ln b|)^2}\right)k^2\,. \tag{6.87}$$

Proof. Replacing x by xk and using the monotonicity of ln we see that it suffices to consider $k=1$. Since $\ln x\geq -\frac{1}{de}x^{-d}$ for all $d>0$ we have

$$\frac{x^2}{b^2}\frac{|\ln b|}{|\ln x|}-2\frac{x}{b}\geq\frac{|\ln b|}{b^2}edx^{2+d}-\frac{2x}{b}\geq c(d)(b^d ed|\ln b|)^{-1/(1+d)} \tag{6.88}$$

with

$$\begin{aligned} c(d)&=2^{(2+d)/(1+d)}\left(\frac{1}{(2+d)^{(2+d)/(1+d)}}-\frac{1}{(2+d)^{1/(1+d)}}\right)\\ &\geq -1-\frac{1}{4}d^2\,. \end{aligned} \tag{6.89}$$

Choosing $d=1/|\ln b|$ gives the desired result. □

Applying this lemma with $x=a^2n_\alpha/L^2$, $b=a^2\rho_{\alpha,\max}$ and

$$k=\frac{\rho_{\alpha,\max}}{\rho_{\alpha,\min}}\left(1-\frac{C}{|\ln(a^2N/L^2)|^{1/5}}\right)^{-1}\frac{|\ln(a^2\rho_{\alpha,\max})|}{|\ln(a^2\bar{\rho}_N)|} \tag{6.90}$$

we get the bound

$$(6.86)\geq -4\pi\frac{\rho_{\alpha,\max}^2L^2}{|\ln(a^2\bar{\rho}_N)|}\left(1+\frac{1}{4|\ln(a^2\rho_{\alpha,\max})|^2}\right)k\,. \tag{6.91}$$

In the limit considered, k and the factor in parenthesis both tend to 1 and the Riemann sum over the boxes α converges to the integral as $L\to 0$.

The TF case, Thm. 6.6, is treated in the same way as in three dimensions, with modifications analogous to those just discussed when passing from 3D to 2D in GP theory.

7 Bose–Einstein Condensation and Superfluidity for Dilute Trapped Gases

It was shown in the previous section that, for each fixed Na, the minimization of the GP functional correctly reproduces the large N asymptotics of the ground state energy and density of H – but no assertion about BEC in this limit was made. We will now extend this result by showing that in the Gross–Pitaevskii limit there is indeed 100% Bose condensation in the ground state. This is a generalization of the homogeneous case considered in Theorem 5.1 and although it is not the same as BEC in the thermodynamic limit it is quite relevant for the actual experiments with Bose gases in traps. In the following, we concentrate on the 3D case, but analogous considerations apply also to the 2D case. We also discuss briefly some extensions of Theorem 5.3 pertaining to superfluidity in trapped gases.

As in the last section we choose to keep the length scale $L_{\rm osc}$ of the confining potential fixed and thus write Na instead of $Na/L_{\rm osc}$. Consequently the powers of N appearing in the proofs are different from those in the proof Theorem 5.1, where we kept Na/L *and* N/L^3 fixed.

For use later, we define the projector

$$P^{\rm GP} = |\phi^{\rm GP}\rangle\langle\phi^{\rm GP}| \, . \tag{7.1}$$

Here (and everywhere else in this section) we denote $\phi^{\rm GP} \equiv \phi^{\rm GP}_{1,Na}$ for simplicity, where $\phi^{\rm GP}_{1,Na}$ is the minimizer of the GP functional (6.2) with parameter Na and normalization condition $\int |\phi|^2 = 1$ (compare with (6.8)). Moreover, we set $\mu \equiv 1$.

In the following, Ψ_0 denotes the (nonnegative and normalized) ground state of the Hamiltonian (6.1). BEC refers to the reduced one-particle density matrix $\gamma(\mathbf{x}, \mathbf{x}')$ of Ψ_0, defined in (5.1). The precise definition of BEC is is that for some $c > 0$ this integral operator has for all large N an an eigenfunction with eigenvalue $\geq cN$.

Complete (or 100%) BEC is defined to be the property that $\frac{1}{N}\gamma(\mathbf{x}, \mathbf{x}')$ not only has an eigenvalue of order one, as in the general case of an incomplete BEC, but in the limit it has only one nonzero eigenvalue (namely 1). Thus, $\frac{1}{N}\gamma(\mathbf{x}, \mathbf{x}')$ becomes a simple product $\varphi(\mathbf{x})^*\varphi(\mathbf{x}')$ as $N \to \infty$, in which case φ is called the *condensate wave function*. In the GP limit, i.e., $N \to \infty$ with Na fixed, we can show that this is the case, and the condensate wave function is, in fact, the GP minimizer $\phi^{\rm GP}$.

Theorem 7.1 (Bose–Einstein condensation in a trap).
For each fixed Na

$$\lim_{N\to\infty} \frac{1}{N}\gamma(\mathbf{x}, \mathbf{x}') = \phi^{\rm GP}(\mathbf{x})\phi^{\rm GP}(\mathbf{x}') \tag{7.2}$$

in trace norm, i.e., $\mathrm{Tr}\left|\frac{1}{N}\gamma - P^{\rm GP}\right| \to 0$.

We remark that Theorem 7.1 implies that there is also 100% condensation for all n-particle reduced density matrices

$$\gamma^{(n)}(\mathbf{x}_1,\dots,\mathbf{x}_n;\mathbf{x}'_1,\dots,\mathbf{x}'_n) = \\ n!\binom{N}{n}\int \Psi_0(\mathbf{x}_1,\dots,\mathbf{x}_N)\Psi_0(\mathbf{x}'_1,\dots,\mathbf{x}'_n,\mathbf{x}_{n+1},\dots\mathbf{x}_N)\mathrm{d}\mathbf{x}_{n+1}\cdots\mathrm{d}\mathbf{x}_N \quad (7.3)$$

of Ψ_0, i.e., they converge, after division by the normalization factor, to the one-dimensional projector onto the n-fold tensor product of ϕ^{GP}. In other words, for n fixed particles the probability of finding them all in the same state ϕ^{GP} tends to 1 in the limit considered. To see this, let a^*, a denote the boson creation and annihilation operators for the state ϕ^{GP}, and observe that

$$1 \geq \lim_{N\to\infty} N^{-n}\langle\Psi_0|(a^*)^n a^n|\Psi_0\rangle = \lim_{N\to\infty} N^{-n}\langle\Psi_0|(a^*a)^n|\Psi_0\rangle\ , \quad (7.4)$$

since the terms coming from the commutators $[a,a^*]=1$ are of lower order as $N\to\infty$ and vanish in the limit. From convexity it follows that

$$N^{-n}\langle\Psi_0|(a^*a)^n|\Psi_0\rangle \geq N^{-n}\langle\Psi_0|a^*a|\Psi_0\rangle^n\ , \quad (7.5)$$

which converges to 1 as $N\to\infty$, proving our claim.

Another corollary, important for the interpretation of experiments, concerns the momentum distribution of the ground state.

Corollary 7.2 (Convergence of momentum distribution). *Let*

$$\widehat{\rho}(\mathbf{k}) = \int\int \gamma(\mathbf{x},\mathbf{x}')\exp[i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')]\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}' \quad (7.6)$$

denote the one-particle momentum density of Ψ_0. Then, for fixed Na,

$$\lim_{N\to\infty}\frac{1}{N}\widehat{\rho}(\mathbf{k}) = |\widehat{\phi}^{\mathrm{GP}}(\mathbf{k})|^2 \quad (7.7)$$

strongly in $L^1(\mathbb{R}^3)$. Here, $\widehat{\phi}^{\mathrm{GP}}$ denotes the Fourier transform of ϕ^{GP}.

Proof. If $\mathcal{F}$ denotes the (unitary) operator 'Fourier transform' and if h is an arbitrary L^∞-function, then

$$\begin{aligned}\left|\frac{1}{N}\int\widehat{\rho}h - \int|\widehat{\phi}^{\mathrm{GP}}|^2 h\right| &= \left|\mathrm{Tr}\,[\mathcal{F}^{-1}(\gamma/N - P^{\mathrm{GP}})\mathcal{F}h]\right| \\ &\leq \|h\|_\infty \mathrm{Tr}\,|\gamma/N - P^{\mathrm{GP}}|\ ,\end{aligned} \quad (7.8)$$

from which we conclude that

$$\|\widehat{\rho}/N - |\widehat{\phi}^{\mathrm{GP}}|^2\|_1 \leq \mathrm{Tr}\,|\gamma/N - P^{\mathrm{GP}}|\ . \quad (7.9)$$

□

As already stated, Theorem 7.1 is a generalization of Theorem 5.1, the latter corresponding to the case that V is a box potential. It should be noted, however, that we use different scaling conventions in these two theorems: In Theorem 5.1 the box size grows as $N^{1/3}$ to keep the density fixed, while in Theorem 7.1 we choose to keep the confining external potential fixed. Both conventions are equivalent, of course, c.f. the remarks in the second paragraph of Sect. 6, but when comparing the exponents of N that appear in the proofs of the two theorems the different conventions should be born in mind.

As in Theorem 5.1 there are two essential components of our proof of Theorem 7.1. The first is a proof that the part of the kinetic energy that is associated with the interaction v (namely, the second term in (6.17a)) is mostly located in small balls surrounding each particle. More precisely, these balls can be taken to have radius roughly $N^{-5/9}$, which is much smaller than the mean-particle spacing $N^{-1/3}$. (The exponents differ from those of Lemma 5.2 because of different scaling conventions.) This allows us to conclude that the function of $\mathbf{x}$ defined for each fixed value of $\mathbf{X}$ by

$$f_{\mathbf{X}}(\mathbf{x}) = \frac{1}{\phi^{\mathrm{GP}}(\mathbf{x})}\Psi_0(\mathbf{x},\mathbf{X}) \geq 0 \tag{7.10}$$

has the property that $\nabla_{\mathbf{x}} f_{\mathbf{X}}(\mathbf{x})$ is almost zero outside the small balls centered at points of $\mathbf{X}$.

The complement of the small balls has a large volume but it can be a weird set; it need not even be connected. Therefore, the smallness of $\nabla_{\mathbf{x}} f_{\mathbf{X}}(\mathbf{x})$ in this set does not guarantee that $f_{\mathbf{X}}(\mathbf{x})$ is nearly constant (in $\mathbf{x}$), or even that it is continuous. We need $f_{\mathbf{X}}(\mathbf{x})$ to be nearly constant in order to conclude BEC. What saves the day is the knowledge that the total kinetic energy of $f_{\mathbf{X}}(\mathbf{x})$ (including the balls) is not huge. The result that allows us to combine these two pieces of information in order to deduce the almost constancy of $f_{\mathbf{X}}(\mathbf{x})$ is the generalized Poincaré inequality in Lemma 4.3. The important point in this lemma is that there is no restriction on Ω concerning regularity or connectivity.

Using the results of Theorem 6.2, partial integration and the GP equation (i.e., the variational equation for ϕ^{GP}, see (6.5)) we see that

$$\lim_{N\to\infty} \int |\phi^{\mathrm{GP}}(\mathbf{x})|^2 |\nabla_{\mathbf{x}} f_{\mathbf{X}}(\mathbf{x})|^2 \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{X} = 4\pi N a s \int |\phi^{\mathrm{GP}}(\mathbf{x})|^4 \mathrm{d}\mathbf{x}\,. \tag{7.11}$$

The following Lemma shows that to leading order all the energy in (7.11) is concentrated in small balls.

Lemma 7.3 (Localization of the energy in a trap). *For fixed* $\mathbf{X}$ *let*

$$\Omega_{\mathbf{X}} = \left\{ \mathbf{x} \in \mathbb{R}^3 \,\middle|\, \min_{k\geq 2} |\mathbf{x} - \mathbf{x}_k| \geq N^{-1/3-\delta} \right\} \tag{7.12}$$

for some $0 < \delta < 2/9$*. Then*

$$\lim_{N\to\infty} \int \mathrm{d}\mathbf{X} \int_{\Omega_{\mathbf{X}}} \mathrm{d}\mathbf{x} |\phi^{\mathrm{GP}}(\mathbf{x})|^2 |\nabla_{\mathbf{x}} f_{\mathbf{X}}(\mathbf{x})|^2 = 0 \,. \tag{7.13}$$

Remark. In the proof of Theorem 5.1 we chose δ to be $4/51$, but the following proof shows that one can extend the range of δ beyond this value.

Proof. We shall show that

$$\begin{aligned} &\int \mathrm{d}\mathbf{X} \int_{\Omega^c_{\mathbf{X}}} \mathrm{d}\mathbf{x}\, |\phi^{\mathrm{GP}}(\mathbf{x})|^2 |\nabla_{\mathbf{x}} f_{\mathbf{X}}(\mathbf{x})|^2 \\ &\quad + \int \mathrm{d}\mathbf{X} \int \mathrm{d}\mathbf{x} |\phi^{\mathrm{GP}}(\mathbf{x})|^2 |f_{\mathbf{X}}(\mathbf{x})|^2 \left[\tfrac{1}{2} \sum_{k\geq 2} v(|\mathbf{x}-\mathbf{x}_k|) - 8\pi N a |\phi^{\mathrm{GP}}(\mathbf{x})|^2 \right] \\ &\qquad \geq -4\pi N a \int |\phi^{\mathrm{GP}}(\mathbf{x})|^4 \mathrm{d}\mathbf{x} - o(1) \end{aligned} \tag{7.14}$$

as $N \to \infty$. We claim that this implies the assertion of the Lemma. To see this, note that the left side of (7.14) can be written as

$$\frac{1}{N} E_0 - \mu^{\mathrm{GP}} - \int \mathrm{d}\mathbf{X} \int_{\Omega_{\mathbf{X}}} \mathrm{d}\mathbf{x} |\phi^{\mathrm{GP}}(\mathbf{x})|^2 |\nabla_{\mathbf{x}} f_{\mathbf{X}}(\mathbf{x})|^2 \,, \tag{7.15}$$

where we used partial integration and the GP equation (6.5), and also the symmetry of Ψ_0. The convergence of the energy in Theorem 6.1 and the relation (6.6) now imply the desired result.

The proof of (7.14) is actually just a detailed examination of the lower bounds to the energy derived in [53] and [62] and described in Sects. 2 and 6. We use the same methods as there, just describing the differences from the case considered here.

Writing

$$f_{\mathbf{X}}(\mathbf{x}) = \prod_{k\geq 2} \phi^{\mathrm{GP}}(\mathbf{x}_k) F(\mathbf{x}, \mathbf{X}) \tag{7.16}$$

and using that F is symmetric in the particle coordinates, we see that (7.14) is equivalent to

$$\frac{1}{N} Q_\delta(F) \geq -4\pi N a \int |\phi^{\mathrm{GP}}|^4 - o(1) \,, \tag{7.17}$$

where Q_δ is the quadratic form

$$\begin{aligned} Q_\delta(F) = &\sum_{i=1}^N \int_{\Omega_i^c} |\nabla_i F|^2 \prod_{k=1}^N |\phi^{\mathrm{GP}}(\mathbf{x}_k)|^2 \mathrm{d}\mathbf{x}_k \\ &+ \sum_{1\leq i<j\leq N} \int v(|\mathbf{x}_i - \mathbf{x}_j|) |F|^2 \prod_{k=1}^N |\phi^{\mathrm{GP}}(\mathbf{x}_k)|^2 \mathrm{d}\mathbf{x}_k \\ &- 8\pi N a \sum_{i=1}^N \int |\phi^{\mathrm{GP}}(\mathbf{x}_i)|^2 |F|^2 \prod_{k=1}^N |\phi^{\mathrm{GP}}(\mathbf{x}_k)|^2 \mathrm{d}\mathbf{x}_k \,. \end{aligned} \tag{7.18}$$

Here Ω_i^c denotes the set

$$\Omega_i^c = \{(\mathbf{x}_1, \mathbf{X}) \in \mathbb{R}^{3N} | \min_{k \neq i} |\mathbf{x}_i - \mathbf{x}_k| \leq N^{-1/3-\delta}\} . \tag{7.19}$$

While (7.17) is not true for all conceivable F's satisfying the normalization condition

$$\int |F(\mathbf{x}, \mathbf{X})|^2 \prod_{k=1}^{N} |\phi^{\mathrm{GP}}(\mathbf{x}_k)|^2 \mathrm{d}\mathbf{x}_k = 1 , \tag{7.20}$$

it *is* true for an F, such as ours, that has bounded kinetic energy (7.11). Looking at Sect. 6, we see that (6.28)–(6.29), (6.48)–(6.52) are similar to (7.17), (7.18) and almost establish (7.17), but there are differences which we now explain.

In our case, the kinetic energy of particle i is restricted to the subset of $\mathbb{R}^{3N}$ in which $\min_{k \neq i} |\mathbf{x}_i - \mathbf{x}_k| \leq N^{-1/3-\delta}$. However, looking at the proof of the lower bound to the ground state energy of a homogeneous Bose gas discussed in Sect. 2, which enters the proof of Theorem 6.1, we see that if we choose $\delta \leq 4/51$ only this part of the kinetic energy is needed for the lower bound, except for some part with a relative magnitude of the order $\varepsilon = O(N^{-2\alpha})$ with $\alpha = 1/17$. (Here we use the a priori knowledge that the kinetic energy is bounded by (7.11).) We can even do better and choose some $4/51 < \delta < 2/9$, if α is chosen small enough. (To be precise, we choose $\beta = 1/3 + \alpha$ and $\gamma = 1/3 - 4\alpha$ in the notation of (2.56), and α small enough). The choice of α only affects the magnitude of the error term, however, which is still $o(1)$ as $N \to \infty$. □

Proof (Theorem 7.1). For some $R > 0$ let $\mathcal{K} = \{\mathbf{x} \in \mathbb{R}^3, |\mathbf{x}| \leq R\}$, and define

$$\langle f_{\mathbf{X}} \rangle_{\mathcal{K}} = \frac{1}{\int_{\mathcal{K}} |\phi^{\mathrm{GP}}(\mathbf{x})|^2 \mathrm{d}\mathbf{x}} \int_{\mathcal{K}} |\phi^{\mathrm{GP}}(\mathbf{x})|^2 f_{\mathbf{X}}(\mathbf{x}) \, \mathrm{d}\mathbf{x} . \tag{7.21}$$

We shall use Lemma 4.3, with $d = 3$, $h(\mathbf{x}) = |\phi^{\mathrm{GP}}(\mathbf{x})|^2 / \int_{\mathcal{K}} |\phi^{\mathrm{GP}}|^2$, $\Omega = \Omega_{\mathbf{X}} \cap \mathcal{K}$ and $f(\mathbf{x}) = f_{\mathbf{X}}(\mathbf{x}) - \langle f_{\mathbf{X}} \rangle_{\mathcal{K}}$ (see (7.12) and (7.10)). Since ϕ^{GP} is bounded on $\mathcal{K}$ above and below by some positive constants, this Lemma also holds (with a different constant C') with $\mathrm{d}\mathbf{x}$ replaced by $|\phi^{\mathrm{GP}}(\mathbf{x})|^2 d\mathbf{x}$ in (4.6). Therefore,

$$\begin{aligned} \int \mathrm{d}\mathbf{X} \int_{\mathcal{K}} \mathrm{d}\mathbf{x} |\phi^{\mathrm{GP}}(\mathbf{x})|^2 \left[f_{\mathbf{X}}(\mathbf{x}) - \langle f_{\mathbf{X}} \rangle_{\mathcal{K}} \right]^2 & \\ \leq C' \int \mathrm{d}\mathbf{X} \Bigg[\int_{\Omega_{\mathbf{X}} \cap \mathcal{K}} & |\phi^{\mathrm{GP}}(\mathbf{x})|^2 |\nabla_{\mathbf{x}} f_{\mathbf{X}}(\mathbf{x})|^2 \mathrm{d}\mathbf{x} \\ + \frac{N^{-2\delta}}{R^2} \int_{\mathcal{K}} & |\phi^{\mathrm{GP}}(\mathbf{x})|^2 |\nabla_{\mathbf{x}} f_{\mathbf{X}}(\mathbf{x})|^2 \mathrm{d}\mathbf{x} \Bigg] , \end{aligned} \tag{7.22}$$

where we used that $|\Omega_{\mathbf{X}}^c \cap \mathcal{K}| \leq (4\pi/3) N^{-3\delta}$. The first integral on the right side of (7.22) tends to zero as $N \to \infty$ by Lemma 7.3, and the second is bounded by (7.11). We conclude, since

$$\int_{\mathcal{K}} |\phi^{\rm GP}(\mathbf{x})|^2 f_{\mathbf{X}}(\mathbf{x}) \mathrm{d}\mathbf{x} \leq \int_{\mathbb{R}^3} |\phi^{\rm GP}(\mathbf{x})|^2 f_{\mathbf{X}}(\mathbf{x}) \mathrm{d}\mathbf{x} \tag{7.23}$$

because of the positivity of $f_{\mathbf{X}}$, that

$$\begin{aligned}\liminf_{N\to\infty} \frac{1}{N}\langle \phi^{\rm GP}|\gamma|\phi^{\rm GP}\rangle &\geq \int_{\mathcal{K}} |\phi^{\rm GP}(\mathbf{x})|^2 \mathrm{d}\mathbf{x} \lim_{N\to\infty} \int \mathrm{d}\mathbf{X} \int_{\mathcal{K}} \mathrm{d}\mathbf{x} |\Psi_0(\mathbf{x},\mathbf{X})|^2 \\ &= \left[\int_{\mathcal{K}} |\phi^{\rm GP}(\mathbf{x})|^2 \mathrm{d}\mathbf{x}\right]^2 ,\end{aligned} \tag{7.24}$$

where the last equality follows from (6.16). Since the radius of $\mathcal{K}$ was arbitrary, we conclude that

$$\lim_{N\to\infty} \frac{1}{N}\langle \phi^{\rm GP}|\gamma|\phi^{\rm GP}\rangle = 1 , \tag{7.25}$$

implying convergence of γ/N to $P^{\rm GP}$ in Hilbert–Schmidt norm. Since the traces are equal, convergence even holds in trace norm (cf. [81], Thm. 2.20), and Theorem 7.1 is proven. □

We remark that the method presented here also works in the case of a two-dimensional Bose gas. The relevant parameter to be kept fixed in the GP limit is $N/|\ln(a^2\bar{\rho}_N)|$, all other considerations carry over without essential change, using the results in [54, 63], c.f. Sects. 3 and 6.2. It should be noted that the existence of BEC in the ground state in 2D is not in conflict with its absence at positive temperatures [33, 66]. In the hard core lattice gas at half filling precisely this phenomenon occurs [38].

Finally, we remark on generalizations of Theorem 5.3 on superfluidity from a torus to some physically more realistic settings. As an example, let $\mathcal{C}$ be a finite cylinder based on an annulus centered at the origin. Given a bounded, real function $a(r,z)$ let A be the vector field (in polar coordinates) $A(r,\theta,z) = \varphi a(r,z)\widehat{e}_\theta$, where $\widehat{e}_\theta$ is the unit vector in the θ direction. We also allow for a bounded external potential $V(r,z)$ that does not depend on θ.

Using the methods of Appendix A in [53], it is not difficult to see that there exists a $\varphi_0 > 0$, depending only on $\mathcal{C}$ and $a(r,z)$, such that for all $|\varphi| < \varphi_0$ there is a unique minimizer $\phi^{\rm GP}$ of the Gross–Pitaevskii functional

$$\mathcal{E}^{\rm GP}[\phi] = \int_{\mathcal{C}} \Big(\big|\big(\nabla + \mathrm{i}A(\mathbf{x})\big)\phi(\mathbf{x})\big|^2 + V(\mathbf{x})|\phi(\mathbf{x})|^2 + 4\pi\mu N a|\phi(\mathbf{x})|^4\Big)\mathrm{d}\mathbf{x} \tag{7.26}$$

under the normalization condition $\int |\phi|^2 = 1$. This minimizer does not depend on θ, and can be chosen to be positive, for the following reason: The relevant term in the kinetic energy is $T = -r^{-2}[\partial/\partial\theta + \mathrm{i}\varphi\, r\, a(r,z)]^2$. If $|\varphi\, r\, a(r,z)| < 1/2$, it is easy to see that $T \geq \varphi^2 a(r,z)^2$, in which case, without raising the energy, we can replace ϕ by the square root of the θ-average of $|\phi|^2$. This can only lower the kinetic energy [49] and, by convexity of $x \to x^2$, this also lowers the ϕ^4 term.

We denote the ground state energy of $\mathcal{E}^{\mathrm{GP}}$ by E^{GP}, depending on Na and φ. The following Theorem 7.4 concerns the ground state energy E_0 of

$$H_N^A = \sum_{j=1}^{N} \Big[-\left(\nabla_j + \mathrm{i}A(\mathbf{x}_j)\right)^2 + V(\mathbf{x}_j)\Big] + \sum_{1\leq i<j\leq N} v(|\mathbf{x}_i - \mathbf{x}_j|)\ , \tag{7.27}$$

with Neumann boundary conditions on $\mathcal{C}$, and the one-particle reduced density matrix γ_N of the ground state, respectively. Different boundary conditions can be treated in the same manner, if they are also used in (7.26).

Remark. As a special case, consider a uniformly rotating system. In this case $A(\mathbf{x}) = \varphi r \widehat{e}_\theta$, where 2φ is the angular velocity. H_N^A is the Hamiltonian in the rotating frame, but with external potential $V(\mathbf{x}) + A(\mathbf{x})^2$ (see e.g. [4, p. 131]).

Theorem 7.4 (Superfluidity in a cylinder). *For* $|\varphi| < \varphi_0$

$$\lim_{N\to\infty} \frac{E_0(N,a,\varphi)}{N} = E^{\mathrm{GP}}(Na,\varphi) \tag{7.28}$$

in the limit $N \to \infty$ *with* Na *fixed. In the same limit,*

$$\lim_{N\to\infty} \frac{1}{N} \gamma_N(\mathbf{x},\mathbf{x}') = \phi^{\mathrm{GP}}(\mathbf{x})\phi^{\mathrm{GP}}(\mathbf{x}') \tag{7.29}$$

in trace class norm, i.e., $\lim_{N\to\infty} \mathrm{Tr}\left[\,\big|\gamma_N/N - |\phi^{\mathrm{GP}}\rangle\langle\phi^{\mathrm{GP}}|\,\big|\,\right] = 0$.

In the case of a uniformly rotating system, where 2φ is the angular velocity, the condition $|\varphi| < \varphi_0$ in particular means that the angular velocity is smaller than the critical velocity for creating vortices [79, 21].

Remark. In the special case of the curl-free vector potential $A(r,\theta) = \varphi r^{-1}\widehat{e}_\theta$, i.e., $a(r,z) = r^{-1}$, one can say more about the role of φ_0. In this case, there is a unique GP minimizer for all $\varphi \notin \mathbb{Z}+\frac{1}{2}$, whereas there are two minimizers for $\varphi \in \mathbb{Z}+\frac{1}{2}$. Part two of Theorem 7.4 holds in this special case for all $\varphi \notin \mathbb{Z}+\frac{1}{2}$, and (7.28) is true even for all φ.

8 One-Dimensional Behavior of Dilute Bose Gases in Traps

Recently it has become possible to do experiments in highly elongated traps on ultra-cold Bose gases that are effectively one-dimensional [8, 27, 29, 76, 65]. These experiments show peculiar features predicted by a model of a one-dimensional Bose gas with repulsive δ-function pair interaction, analyzed long ago by Lieb and Liniger [48]. These include quasi-fermionic behavior [24], the absence of Bose–Einstein condensation (BEC) in a dilute limit [43, 72, 26], and an excitation spectrum different from that predicted by Bogoliubov's theory [48, 37, 42]. The theoretical work on the dimensional cross-over for the ground state in elongated traps has so far been based either on variational calculations, starting from a 3D delta-potential [67, 15, 25], or on numerical Quantum Monte Carlo studies [6, 1] with more realistic, genuine 3D potentials, but particle numbers limited to the order of 100. This work is important and has led to valuable insights, in particular about different parameter regions [70, 16], but a more thorough theoretical understanding is clearly desirable since this is not a simple problem. In fact, it is evident that for a potential with a hard core the true 3D wave functions do not approximately factorize in the longitudinal and transverse variables (otherwise the energy would be infinite) and the effective 1D potential can not be obtained by simply integrating out the transverse variables of the 3D potential (that would immediately create an impenetrable barrier in 1D). It is important to be able to demonstrate rigorously, and therefore unambiguously, that the 1D behavior really follows from the fundamental Schrödinger equation. It is also important to delineate, as we do here, precisely what can be seen in the different parameter regions. The full proofs of our assertions are long and are given in [58]. Here we state our main results and outline the basic ideas for the proofs.

We start by describing the setting more precisely. It is convenient to write the Hamiltonian in the following way (in units where $\hbar = 2m = 1$):

$$H_{N,L,r,a} = \sum_{j=1}^{N} \left(-\Delta_j + V_r^{\perp}(\mathbf{x}_j^{\perp}) + V_L(z_j)\right) + \sum_{1\leq i<j\leq N} v_a(|\mathbf{x}_i - \mathbf{x}_j|) \tag{8.1}$$

with $\mathbf{x} = (x, y, z) = (\mathbf{x}^{\perp}, z)$ and with

$$\begin{gathered} V_r^{\perp}(\mathbf{x}^{\perp}) = \frac{1}{r^2} V^{\perp}(\mathbf{x}^{\perp}/r) , \\ V_L(z) = \frac{1}{L^2} V(z/L) , \quad v_a(|\mathbf{x}|) = \frac{1}{a^2} v(|\mathbf{x}|/a) . \end{gathered} \tag{8.2}$$

Here, r, L, a are variable scaling parameters while $V^{\perp}$, V and v are fixed.

We shall be concerned with the ground state of this Hamiltonian for large particle number N, which is appropriate for the consideration of actual experiments. The other parameters of the problem are the scattering length, a, of the two-body interaction potential, v, and two lengths, r and L, describing the transverse and the longitudinal extension of the trap potential, respectively.

The interaction potential v is supposed to be nonnegative, of finite range and have scattering length 1; the scaled potential v_a then has scattering length a. The external trap potentials V and $V^{\perp}$ confine the motion in the longitudinal (z) and the transversal ($\mathbf{x}^{\perp}$) directions, respectively, and are assumed to be continuous and tend to ∞ as $|z|$ and $|\mathbf{x}^{\perp}|$ tend to ∞. To simplify the discussion we find it also convenient to assume that V is homogeneous of some order $s > 0$, namely $V(z) = |z|^s$, but weaker assumptions, e.g. asymptotic homogeneity (cf. Sect. 6), would in fact suffice. The case of a simple box with hard walls is realized by taking $s = \infty$, while the usual harmonic approximation is $s = 2$. It is understood that the lengths associated with the ground states of $-\mathrm{d}^2/\mathrm{d}z^2 + V(z)$ and $-\Delta^\perp + V^\perp(\mathbf{x}^\perp)$ are both of the order 1 so that L and r measure, respectively, the longitudinal and the transverse extensions of the trap. We denote the ground state energy of (8.1) by $E^{\mathrm{QM}}(N, L, r, a)$ and the ground state particle density by $\rho^{\mathrm{QM}}_{N,L,r,a}(\mathbf{x})$. On the average, this 3D density will always be low in the parameter range considered here (in the sense that distance between particles is large compared to the 3D scattering length). The effective 1D density can be either high or low, however.

In parallel with the 3D Hamiltonian we consider the Hamiltonian for n Bosons in 1D with delta interaction and coupling constant $g \geq 0$, i.e.,

$$H^{\mathrm{1D}}_{n,g} = \sum_{j=1}^{n} -\partial^2/\partial z_j^2 + g \sum_{1\leq i<j\leq n} \delta(z_i - z_j) \ . \tag{8.3}$$

We consider this Hamiltonian for the z_j in an interval of length ℓ in the thermodynamic limit, $\ell \to \infty$, $n \to \infty$ with $\rho = n/\ell$ fixed. The ground state energy per particle in this limit is independent of boundary conditions and can, according to [48], be written as

$$e_0^{\mathrm{1D}}(\rho) = \rho^2 e(g/\rho) \ , \tag{8.4}$$

with a function $e(t)$ determined by a certain integral equation. Its asymptotic form is $e(t) \approx \frac{1}{2}t$ for $t \ll 1$ and $e(t) \to \pi^2/3$ for $t \to \infty$. Thus

$$e_0^{\mathrm{1D}}(\rho) \approx \tfrac{1}{2} g\rho \quad \text{for} \quad g/\rho \ll 1 \tag{8.5}$$

and

$$e_0^{\mathrm{1D}}(\rho) \approx (\pi^2/3)\rho^2 \quad \text{for} \quad g/\rho \gg 1 \ . \tag{8.6}$$

This latter energy is the same as for non-interacting fermions in 1D, which can be understood from the fact that (8.3) with $g = \infty$ is equivalent to a Hamiltonian describing free fermions.

Taking $\rho e_0^{\mathrm{1D}}(\rho)$ as a local energy density for an inhomogeneous 1D system we can form the energy functional

$$\mathcal{E}[\rho] = \int_{-\infty}^{\infty} \left(|\nabla\sqrt{\rho}(z)|^2 + V_L(z)\rho(z) + \rho(z)^3 e(g/\rho(z)) \right) \mathrm{d}z \ . \tag{8.7}$$

Its ground state energy is obtained by minimizing over all normalized densities, i.e.,

$$E^{\mathrm{1D}}(N, L, g) = \inf \left\{ \mathcal{E}[\rho] \ : \ \rho(z) \geq 0, \int_{-\infty}^{\infty} \rho(z)\mathrm{d}z = N \right\} \ . \tag{8.8}$$

Using convexity of the map $\rho \mapsto \rho^3 e(g/\rho)$, it is standard to show that there exists a unique minimizer of (8.7) (see, e.g., [53]). It will be denoted by $\rho_{N,L,g}$. We also define the *mean 1D density* of this minimizer to be

$$\bar{\rho} = \frac{1}{N} \int_{-\infty}^{\infty} (\rho_{N,L,g}(z))^2 \, \mathrm{d}z \ . \tag{8.9}$$

In a rigid box, i.e., for $s = \infty$, $\bar{\rho}$ is simply N/L (except for boundary corrections), but in more general traps it depends also on g besides N and L. The order of magnitude of $\bar{\rho}$ in the various parameter regions will be described below.

Our main result relates the 3D ground state energy of (8.1) to the 1D density functional energy $E^{1\mathrm{D}}(N, L, g)$ in the large N limit with $g \sim a/r^2$ provided r/L and a/r are sufficiently small. To state this precisely, let $e^{\perp}$ and $b(\mathbf{x}^{\perp})$, respectively, denote the ground state energy and the normalized ground state wave function of $-\Delta^{\perp} + V^{\perp}(\mathbf{x}^{\perp})$. The corresponding quantities for $-\Delta^{\perp} + V_r^{\perp}(\mathbf{x}^{\perp})$ are $e^{\perp}/r^2$ and $b_r(\mathbf{x}^{\perp}) = (1/r)b(\mathbf{x}^{\perp}/r)$. In the case that the trap is a cylinder with hard walls b is a Bessel function; for a quadratic $V^{\perp}$ it is a Gaussian.

Define g by

$$g = \frac{8\pi a}{r^2} \int |b(\mathbf{x}^{\perp})|^4 \mathrm{d}\mathbf{x}^{\perp} = 8\pi a \int |b_r(\mathbf{x}^{\perp})|^4 \mathrm{d}\mathbf{x}^{\perp} \ . \tag{8.10}$$

Our main result of this section is:

Theorem 8.1 (From 3D to 1D). *Let $N \to \infty$ and simultaneously $r/L \to 0$ and $a/r \to 0$ in such a way that $r^2\bar{\rho} \times \min\{\bar{\rho}, g\} \to 0$. Then*

$$\lim \frac{E^{\mathrm{QM}}(N, L, r, a) - Ne^{\perp}/r^2}{E^{1\mathrm{D}}(N, L, g)} = 1 \ . \tag{8.11}$$

An analogous result hold for the ground state density. Define the 1D QM density by averaging over the transverse variables, i.e.,

$$\hat{\rho}^{\mathrm{QM}}_{N,L,r,a}(z) \equiv \int \rho^{\mathrm{QM}}_{N,L,r,a}(\mathbf{x}^{\perp}, z) \mathrm{d}\mathbf{x}^{\perp} \ . \tag{8.12}$$

Let $\bar{L} := N/\bar{\rho}$ denote the extension of the system in z-direction, and define the rescaled density $\widetilde{\rho}$ by

$$\rho^{1\mathrm{D}}_{N,L,g}(z) = \frac{N}{\bar{L}} \widetilde{\rho}(z/\bar{L}) \ . \tag{8.13}$$

Note that, although $\widetilde{\rho}$ depends on N, L and g, $\|\widetilde{\rho}\|_1 = \|\widetilde{\rho}\|_2 = 1$, which shows in particular that $\bar{L}$ is the relevant scale in z-direction. The result for the ground state density is:

Theorem 8.2 (1D limit for density). *In the same limit as considered in Theorem 8.1,*

$$\lim \left(\frac{\bar{L}}{N} \hat{\rho}^{\mathrm{QM}}_{N,L,r,a}(z\bar{L}) - \widetilde{\rho}(z) \right) = 0 \tag{8.14}$$

in weak L^1 sense.

Note that because of (8.5) and (8.6) the condition $r^2\bar{\rho} \times \min\{\bar{\rho}, g\} \to 0$ is the same as

$$e_0^{1\mathrm{D}}(\bar{\rho}) \ll 1/r^2 \ , \tag{8.15}$$

i.e., the average energy per particle associated with the longitudinal motion should be much smaller than the energy gap between the ground and first excited state of the confining Hamiltonian in the transverse directions. Thus, the basic physics is highly quantum-mechanical and has no classical counterpart. The system can be described by a 1D functional (8.7), *even though the transverse trap dimension is much larger than the range of the atomic forces.*

8.1 Discussion of the Results

We will now give a discussion of the various parameter regions that are included in the limit considered in Theorems 8.1 and 8.2 above. We begin by describing the division of the space of parameters into two basic regions. This decomposition will eventually be refined into five regions, but for the moment let us concentrate on the basic dichotomy.

In Sect. 6 we proved that the 3D Gross–Pitaevskii formula for the energy is correct to leading order in situations in which N is large but a is small compared to the mean particle distance. This energy has two parts: The energy necessary to confine the particles in the trap, plus the internal energy of interaction, which is $N4\pi a\rho^{3\mathrm{D}}$. This formula was proved to be correct for a *fixed* confining potential in the limit $N \to \infty$ with $a^3\rho^{3\mathrm{D}} \to 0$. However, this limit does not hold uniformly if r/L gets small as N gets large. In other words, new physics can come into play as $r/L \to 0$ and it turns out that this depends on the ratio of a/r^2 to the 1D density, or, in other words, on $g/\bar{\rho}$. There are two basic regimes to consider in highly elongated traps, i.e., when $r \ll L$. They are

- The 1D limit of the 3D Gross–Pitaevskii regime
- The ‘true’ 1D regime.

The former is characterized by $g/\bar{\rho} \ll 1$, while in the latter regime $g/\bar{\rho}$ is of the order one or even tends to infinity. (If $g/\bar{\rho} \to \infty$ the particles are effectively impenetrable; this is usually referred to as the Girardeau–Tonks region.) These two situations correspond to high 1D density (weak interaction) and low 1D density (strong interaction), respectively. Physically, the main difference is that in the strong interaction regime the motion of the particles in the longitudinal direction is highly correlated, while in the weak interaction regime it is not. Mathematically, this distinction also shows up in our proofs. The first region is correctly described by both the 3D and 1D theories because the two give the same predictions there. That’s why we call the second region the ‘true’ 1D regime.

In both regions the internal energy of the gas is small compared to the energy of confinement. However, this in itself does not imply a specifically

1D behavior. (If a is sufficiently small it is satisfied in a trap of any shape.) 1D behavior, when it occurs, manifests itself by the fact that the transverse motion of the atoms is uncorrelated while the longitudinal motion is correlated (very roughly speaking) in the same way as pearls on a necklace. Thus, the true criterion for 1D behavior is that $g/\bar{\rho}$ is of order unity or larger and not merely the condition that the energy of confinement dominates the internal energy.

We shall now briefly describe the finer division of these two regimes into five regions altogether. Three of them (Regions 1–3) belong to the weak interaction regime and two (Regions 4–5) to the strong interaction regime. They are characterized by the behavior of $g/\bar{\rho}$ as $N \to \infty$. In each of these regions the general functional (8.7) can be replaced by a different, simpler functional, and the energy $E^{1\mathrm{D}}(N, L, g)$ in Theorem 8.1 by the ground state energy of that functional. Analogously, the density in Theorem 8.2 can be replaced by the minimizer of the functional corresponding to the region considered.

The five regions are

• **Region 1, the Ideal Gas case:** In the trivial case where the interaction is so weak that it effectively vanishes in the large N limit and everything collapses to the ground state of $-\mathrm{d}^2/\mathrm{d}z^2 + V(z)$ with ground state energy $e^{\|}$, the energy $E^{1\mathrm{D}}$ in (8.11) can be replaced by $Ne^{\|}/L^2$. This is the case if $g/\bar{\rho} \ll N^{-2}$, and the mean density is just $\bar{\rho} \sim N/L$. Note that $g/\bar{\rho} \ll N^{-2}$ means that the 3D interaction energy per particle $\sim a\rho^{3\mathrm{D}} \ll 1/L^2$.

• **Region 2, the 1D GP case:** In this region $g/\bar{\rho} \sim N^{-2}$, with $\bar{\rho} \sim N/L$. This case is described by a 1D Gross–Pitaevskii energy functional of the form

$$\mathcal{E}^{\mathrm{GP}}[\rho] = \int_{-\infty}^{\infty} \left(|\nabla\sqrt{\rho}(z)|^2 + V_L(z)\rho(z) + \tfrac{1}{2}g\rho(z)^2\right) \mathrm{d}z \; , \tag{8.16}$$

corresponding to the high density approximation (8.5) of the interaction energy in (8.7). Its ground state energy, E^{GP}, fulfills the scaling relation $E^{\mathrm{GP}}(N, L, g) = NL^{-2}E^{\mathrm{GP}}(1, 1, NgL)$.

• **Region 3, the 1D TF case:** $N^{-2} \ll g/\bar{\rho} \ll 1$, with $\bar{\rho}$ being of the order $\bar{\rho} \sim (N/L)(NgL)^{-1/(s+1)}$, where s is the degree of homogeneity of the longitudinal confining potential V. This region is described by a Thomas–Fermi type functional

$$\mathcal{E}^{\mathrm{TF}}[\rho] = \int_{-\infty}^{\infty} \left(V_L(z)\rho(z) + \tfrac{1}{2}g\rho(z)^2\right) \mathrm{d}z \; . \tag{8.17}$$

It is a limiting case of Region 2 in the sense that $NgL \gg 1$, but a/r is sufficiently small so that $g/\bar{\rho} \ll 1$, i.e., the high density approximation in (8.5) is still valid. The explanation of the factor $(NgL)^{1/(s+1)}$ is as follows: The linear extension $\bar{L}$ of the minimizing density of (8.16) is for large values of NgL determined by $V_L(\bar{L}) \sim g(N/\bar{L})$, which gives $\bar{L} \sim (NgL)^{1/(s+1)}L$. In addition condition (8.15) requires $g\bar{\rho} \ll r^{-2}$, which means that $Na/L(NgL)^{1/(s+1)} \ll$

1. The minimum energy of (8.17) has the scaling property $E^{\rm TF}(N,L,g) = NL^{-2}(NgL)^{s/(s+1)}E^{\rm TF}(1,1,1)$.

• **Region 4, the LL case:** $g/\bar\rho \sim 1$, with $\bar\rho \sim (N/L)N^{-2/(s+2)}$, described by an energy functional

$$\mathcal{E}^{\rm LL}[\rho] = \int_{-\infty}^{\infty} \big(V_L(z)\rho(z) + \rho(z)^3 e(g/\rho(z))\big)\, {\rm d}z \ . \tag{8.18}$$

This region corresponds to the case $g/\bar\rho \sim 1$, so that neither the high density (8.5) nor the low density approximation (8.6) is valid and the full LL energy (8.4) has to be used. The extension $\bar L$ of the system is now determined by $V_L(\bar L) \sim (N/\bar L)^2$ which leads to $\bar L \sim LN^{2/(s+2)}$. Condition (8.15) means in this region that $Nr/\bar L \sim N^{s/(s+2)}r/L \to 0$. Since $Nr/\bar L \sim (\bar\rho/g)(a/r)$, this condition is automatically fulfilled if $g/\bar\rho$ is bounded away from zero and $a/r \to 0$. The ground state energy of (8.18), $E^{\rm LL}(N,L,g)$, is equal to $N\gamma^2 E^{\rm LL}(1,1,g/\gamma)$, where we introduced the density parameter $\gamma := (N/L)N^{-2/(s+2)}$.

• **Region 5, the GT case:** $g/\bar\rho \gg 1$, with $\bar\rho \sim (N/L)N^{-2/(s+2)}$, described by a functional with energy density $\sim \rho^3$, corresponding to the Girardeau–Tonks limit of the LL energy density. It corresponds to impenetrable particles, i.e, the limiting case $g/\bar\rho \to \infty$ and hence formula (8.6) for the energy density. As in Region 4, the mean density is here $\bar\rho \sim \gamma$. The energy functional is

$$\mathcal{E}^{\rm GT}[\rho] = \int_{-\infty}^{\infty} \big(V_L(z)\rho(z) + (\pi^2/3)\rho(z)^3\big)\, {\rm d}z \ , \tag{8.19}$$

with minimum energy $E^{\rm GT}(N,L) = N\gamma^2 E^{\rm GT}(1,1)$.

As already mentioned above, Regions 1–3 can be reached as limiting cases of a 3D Gross–Pitaevskii theory. In this sense, the behavior in these regions contains remnants of the 3D theory, which also shows up in the fact that BEC prevails in Regions 1 and 2 (See [58] for details.) Heuristically, these traces of 3D can be understood from the fact that in Regions 1–3 the 1D formula for energy per particle, $g\rho \sim aN/(r^2L)$, gives the same result as the 3D formula, i.e., scattering length times 3D density. This is no longer so in Regions 4 and 5 and different methods are required.

8.2 Outline of Proof

We now outline the main steps in the proof of Theorems 8.1 and 8.2, referring to [58] for full details. To prove (8.11) one has to establish upper and lower bounds, with controlled errors, on the QM many-body energy in terms of the energies obtained by minimizing the energy functionals appropriate for the various regions. The limit theorem for the densities can be derived from the energy estimates in a standard way by variation with respect to the external potential V_L.

The different parameter regions have to be treated by different methods, a watershed lying between Regions 1–3 on the one hand and Regions 4–5 on the other. In Regions 1–3, similar methods as in the proof of the 3D Gross–Pitaevskii limit theorem discussed in Sect. 6 can be used. This 3D proof needs some modifications, however, because there the external potential was fixed and the estimates are not uniform in the ratio r/L. We will not go into the details here, but mainly focus on Regions 4 and 5, where new methods are needed. It turns out to be necessary to localize the particles by dividing the trap into finite 'boxes' (finite in z-direction), with a controllable particle number in each box. The particles are then distributed optimally among the boxes to minimize the energy, in a similar way as (2.52) was derived from (2.47).

A core lemma for Regions 4–5 is an estimate of the 3D ground state energy in a finite box in terms of the 1D energy of the Hamiltonian (8.3). I.e., we will consider the ground state energy of (8.1) with the external potential $V_L(z)$ replaced by a finite box (in z-direction) with length ℓ. Let $E_{\mathrm{D}}^{\mathrm{QM}}(n,\ell,r,a)$ and $E_{\mathrm{N}}^{\mathrm{QM}}(n,\ell,r,a)$ denote its ground state energy with Dirichlet and Neumann boundary conditions, respectively.

Lemma 8.3. *Let* $E_{\mathrm{D}}^{\mathrm{1D}}(n,\ell,g)$ *and* $E_{\mathrm{N}}^{\mathrm{1D}}(n,\ell,g)$ *denote the ground state energy of* (8.3) *on* $L^2([0,\ell]^n)$*, with Dirichlet and Neumann boundary conditions, respectively, and let* g *be given by* (8.10)*. Then there is a finite number* $C>0$ *such that*

$$\begin{aligned} E_{\mathrm{N}}^{\mathrm{QM}}(n,\ell,r,a) - \frac{ne^{\perp}}{r^2} \geq E_{\mathrm{N}}^{\mathrm{1D}}(n,\ell,g) \\ \times\left(1 - Cn\left(\frac{a}{r}\right)^{1/8}\left[1+\frac{nr}{\ell}\left(\frac{a}{r}\right)^{1/8}\right]\right) . \end{aligned} \tag{8.20}$$

Moreover,

$$\begin{aligned} E_{\mathrm{D}}^{\mathrm{QM}}(n,\ell,r,a) - \frac{ne^{\perp}}{r^2} \leq E_{\mathrm{D}}^{\mathrm{1D}}(n,\ell,g) \\ \times\left(1 + C\left[\left(\frac{na}{r}\right)^2\left(1+\frac{a\ell}{r^2}\right)\right]^{1/3}\right) , \end{aligned} \tag{8.21}$$

provided the term in square brackets is less than 1.

This Lemma is the key to the proof of Theorems 8.1 and 8.2. The reader interested in the details is referred to [58]. Here we only give a sketch of the proof of Lemma 8.3.

Proof (Lemma 8.3). We start with the upper bound (8.21). Let ψ denote the ground state of (8.3) with Dirichlet boundary conditions, normalized by $\langle\psi|\psi\rangle = 1$, and let $\rho_\psi^{(2)}$ denote its two-particle density, normalized by $\int \rho_\psi^{(2)}(z,z')\mathrm{d}z\mathrm{d}z' = 1$. Let G and F be given by $G(\mathbf{x}_1,\ldots,\mathbf{x}_n) =$

$\psi(z_1,\ldots,z_n)\prod_{j=1}^n b_r(\mathbf{x}_j^\perp)$ and $F(\mathbf{x}_1,\ldots,\mathbf{x}_n)=\prod_{i<j}f(|\mathbf{x}_i-\mathbf{x}_j|)$. Here f is a monotone increasing function, with $0\leq f\leq 1$ and $f(t)=1$ for $t\geq R$ for some $R\geq R_0$. For $t\leq R$ we shall choose $f(t)=f_0(t)/f_0(R)$, where f_0 is the solution to the zero-energy scattering equation for v_a (2.3). Note that $f_0(R)=1-a/R$ for $R\geq R_0$, and $f_0'(t)\leq t^{-1}\min\{1,a/t\}$. We use as a trial wave function

$$\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_n)=G(\mathbf{x}_1,\ldots,\mathbf{x}_n)F(\mathbf{x}_1,\ldots,\mathbf{x}_n)\,. \tag{8.22}$$

We first have to estimate the norm of Ψ. Using the fact that F is 1 whenever no pair of particles is closer together than a distance R, we obtain

$$\langle\Psi|\Psi\rangle\geq 1-\frac{n(n-1)}{2}\frac{\pi R^2}{r^2}\|b\|_4^4\,. \tag{8.23}$$

To evaluate the expectation value of the Hamiltonian, we use

$$\langle\Psi|-\Delta_j|\Psi\rangle=-\int F^2G\Delta_jG+\int G^2|\nabla_jF|^2 \tag{8.24}$$

and the Schrödinger equation $H_{n,g}\psi=E_{\rm D}^{\rm 1D}\psi$. This gives

$$\begin{aligned}\langle\Psi|H|\Psi\rangle&=\left(E_{\rm D}^{\rm 1D}+\frac{n}{r^2}e^\perp\right)\langle\Psi|\Psi\rangle-g\langle\Psi|\sum_{i<j}\delta(z_i-z_j)|\Psi\rangle\\&\quad+\int G^2\left(\sum_{j=1}^n|\nabla_jF|^2+\sum_{i<j}v_a(|\mathbf{x}_i-\mathbf{x}_j|)|F|^2\right)\,.\end{aligned} \tag{8.25}$$

Now, since $0\leq f\leq 1$ and $f'\geq 0$ by assumption, $F^2\leq f(|\mathbf{x}_i-\mathbf{x}_j|)^2$, and

$$\sum_{j=1}^n|\nabla_jF|^2\leq 2\sum_{i<j}f'(|\mathbf{x}_i-\mathbf{x}_j|)^2+4\sum_{k<i<j}f'(|\mathbf{x}_k-\mathbf{x}_i|)f'(|\mathbf{x}_k-\mathbf{x}_j|)\,. \tag{8.26}$$

Consider the first term on the right side of (8.26), together with the last term in (8.25). These terms are bounded above by

$$n(n-1)\int b_r(\mathbf{x}^\perp)^2b_r(\mathbf{y}^\perp)^2\rho_\psi^{(2)}(z,z')\left(f'(|\mathbf{x}-\mathbf{y}|)^2+\tfrac12 v_a(|\mathbf{x}-\mathbf{y}|)f(|\mathbf{x}-\mathbf{y}|)^2\right)\,. \tag{8.27}$$

Let

$$h(z)=\int\left(f'(|\mathbf{x}|)^2+\tfrac12 v_a(|\mathbf{x}|)f(|\mathbf{x}|)^2\right)\mathrm{d}\mathbf{x}^\perp\,. \tag{8.28}$$

Using Young's inequality for the integration over the $\perp$-variables, we get

$$(8.27)\leq\frac{n(n-1)}{r^2}\|b\|_4^4\int_{\mathbb{R}^2}\rho_\psi^{(2)}(z,z')h(z-z')\mathrm{d}z\mathrm{d}z'\,. \tag{8.29}$$

By similar methods, one can show that the contribution from the last term in (8.26) is bounded by

$$\frac{2}{3}n(n-1)(n-2)\frac{\|b\|_\infty^2}{r^2}\frac{\|b\|_4^4}{r^2}\|k\|_\infty \int_{\mathbb{R}^2} \rho_\psi^{(2)}(z,z')k(z-z')\mathrm{d}z\mathrm{d}z' \,, \tag{8.30}$$

where

$$k(z) = \int f'(|\mathbf{x}|)\mathrm{d}\mathbf{x}^\perp \,. \tag{8.31}$$

Note that both h and k are supported in $[-R,R]$.

Now, for any $\phi \in H^1(\mathbb{R})$,

$$\left||\phi(z)|^2 - |\phi(z')|^2\right| \le 2|z-z'|^{1/2}\left(\int_{\mathbb{R}} |\phi|^2\right)^{1/4}\left(\int_{\mathbb{R}} \left|\frac{\mathrm{d}\phi}{\mathrm{d}z}\right|^2\right)^{3/4} \,. \tag{8.32}$$

Applying this to $\rho_\psi^{(2)}(z,z')$, considered as a function of z only, we get

$$\begin{aligned}\int_{\mathbb{R}^2} \rho_\psi^{(2)}(z,z')h(z-z')\mathrm{d}z\mathrm{d}z' - \int_{\mathbb{R}} h(z)\mathrm{d}z \int \rho_\psi^{(2)}(z,z)\mathrm{d}z& \\ \le 2R^{1/2}\int_{\mathbb{R}} h(z)\mathrm{d}z \left\langle \psi\left|-\frac{\mathrm{d}^2}{\mathrm{d}z_1^2}\right|\psi\right\rangle^{3/4} \,,&\end{aligned} \tag{8.33}$$

where we used Schwarz's inequality, the normalization of $\rho_\psi^{(2)}$ and the symmetry of ψ. The same argument is used for (8.30) with h replaced by k.

It remains to bound the second term in (8.25). As in the estimate for the norm of Ψ, we use again the fact that F is equal to 1 as long as the particles are not within a distance R. We obtain

$$\langle\Psi|\sum_{i<j}\delta(z_i-z_j)|\Psi\rangle \ge \frac{n(n-1)}{2}\int \rho_\psi^{(2)}(z,z)\mathrm{d}z\left(1 - \frac{n(n-1)}{2}\frac{\pi R^2}{r^2}\|b\|_4^4\right) \,. \tag{8.34}$$

We also estimate $g\frac{1}{2}n(n-1)\int \rho_\psi^{(2)}(z,z)\mathrm{d}z \le E_{\mathrm{D}}^{1\mathrm{D}}$ and $\langle\psi| - \mathrm{d}^2/\mathrm{d}z_1^2|\psi\rangle \le E_{\mathrm{D}}^{1\mathrm{D}}/n$. We have $\int h(z)\mathrm{d}z = 4\pi a(1-a/R)^{-1}$, and the terms containing k can be bounded by $\|k\|_\infty \le 2\pi a(1+\ln(R/a))/(1-a/r)$ and $\int k(z)\mathrm{d}z \le 2\pi aR(1-a/(2R))/(1-a/r)$. Putting together all the bounds, and choosing

$$R^3 = \frac{ar^2}{n^2(1+g\ell)} \,, \tag{8.35}$$

this proves the desired result.

We are left with the lower bound (8.20). We write a general wave function Ψ as

$$\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_n) = f(\mathbf{x}_1,\ldots,\mathbf{x}_n)\prod_{k=1}^n b_r(\mathbf{x}_k^\perp) \,, \tag{8.36}$$

which can always be done, since b_r is a strictly positive function. Partial integration gives

$$\langle\Psi|H|\Psi\rangle =$$
$$\frac{ne^\perp}{r^2} + \sum_{i=1}^n \int \left[|\nabla_i f|^2 + \tfrac{1}{2} \sum_{j,\, j\neq i} v_a(|\mathbf{x}_i - \mathbf{x}_j|)|f|^2 \right] \prod_{k=1}^n b_r(\mathbf{x}_k^\perp)^2 \mathrm{d}\mathbf{x}_k \,. \quad (8.37)$$

Choose some $R > R_0$, fix i and $\mathbf{x}_j$, $j \neq i$, and consider the Voronoi cell Ω_j around particle j, i.e., $\Omega_j = \{\mathbf{x} : |\mathbf{x} - \mathbf{x}_j| \leq |\mathbf{x} - \mathbf{x}_k| \text{ for all } k \neq j\}$. If $\mathcal{B}_j$ denotes the ball of radius R around $\mathbf{x}_j$, we can estimate with the aid of Lemma 2.5

$$\int_{\Omega_j \cap \mathcal{B}_j} b_r(\mathbf{x}_i^\perp)^2 \left(|\nabla_i f|^2 + \tfrac{1}{2} v_a(|\mathbf{x}_i - \mathbf{x}_j|)|f|^2 \right) \mathrm{d}\mathbf{x}_i$$
$$\geq \frac{\min_{\mathbf{x}\in\mathcal{B}_j} b_r(\mathbf{x}^\perp)^2}{\max_{\mathbf{x}\in\mathcal{B}_j} b_r(\mathbf{x}^\perp)^2} a \int_{\Omega_j \cap \mathcal{B}_j} b_r(\mathbf{x}_i^\perp)^2 U(|\mathbf{x}_i - \mathbf{x}_j|)|f|^2 \,. \quad (8.38)$$

Here U is given in (2.30). For some $\delta > 0$ let $\mathcal{B}_\delta$ be the subset of $\mathbb{R}^2$ where $b(\mathbf{x}^\perp)^2 \geq \delta$, and let $\chi_{\mathcal{B}_\delta}$ denote its characteristic function. Estimating $\max_{\mathbf{x}\in\mathcal{B}_j} b_r(\mathbf{x}^\perp)^2 \leq \min_{\mathbf{x}\in\mathcal{B}_j} b_r(\mathbf{x}^\perp)^2 + 2(R/r^3)\|\nabla b^2\|_\infty$, we obtain

$$\frac{\min_{\mathbf{x}\in\mathcal{B}_j} b_r(\mathbf{x}^\perp)^2}{\max_{\mathbf{x}\in\mathcal{B}_j} b_r(\mathbf{x}^\perp)^2} \geq \chi_{\mathcal{B}_\delta}(\mathbf{x}_j^\perp/r) \left(1 - 2\frac{R}{r}\frac{\|\nabla b^2\|_\infty}{\delta} \right) . \quad (8.39)$$

Denoting $k(i)$ the nearest neighbor to particle i, we conclude that, for $0 \leq \varepsilon \leq 1$,

$$\sum_{i=1}^n \int \left[|\nabla_i f|^2 + \tfrac{1}{2} \sum_{j,\, j\neq i} v_a(|\mathbf{x}_i - \mathbf{x}_j|)|f|^2 \right] \prod_{k=1}^n b_r(\mathbf{x}_k^\perp)^2 \mathrm{d}\mathbf{x}_k$$
$$\geq \sum_{i=1}^n \int \Big[\varepsilon|\nabla_i f|^2 + (1-\varepsilon)|\nabla_i f|^2 \chi_{\min_k |z_i - z_k| \geq R}(z_i) \quad (8.40)$$
$$+ a' U(|\mathbf{x}_i - \mathbf{x}_{k(i)}|)\chi_{\mathcal{B}_\delta}(\mathbf{x}_{k(i)}^\perp/r)|f|^2 \Big] \prod_{k=1}^n b_r(\mathbf{x}_k^\perp)^2 \mathrm{d}\mathbf{x}_k \,,$$

where $a' = a(1-\varepsilon)(1 - 2R\|\nabla b^2\|_\infty/r\delta)$.

Define $F(z_1, \ldots, z_n) \geq 0$ by

$$|F(z_1, \ldots, z_n)|^2 = \int |f(\mathbf{x}_1, \ldots, \mathbf{x}_n)|^2 \prod_{k=1}^n b_r(\mathbf{x}_k^\perp)^2 \mathrm{d}\mathbf{x}_k^\perp \,. \quad (8.41)$$

Neglecting the kinetic energy in $\perp$-direction in the second term in (8.40) and using the Schwarz inequality to bound the longitudinal kinetic energy of f by the one of F, we get the estimate

$$\begin{aligned}\langle\Psi|H|\Psi\rangle - \frac{ne^\perp}{r^2} \\ \geq \sum_{i=1}^n \int \Big[\varepsilon|\partial_i F|^2 + (1-\varepsilon)|\partial_i F|^2 \chi_{\min_k |z_i - z_k| \geq R}(z_i)\Big] \prod_{k=1}^n \mathrm{d}z_k \\ + \sum_{i=1}^n \int \Big[\varepsilon|\nabla_i^\perp f|^2 + a'U(|\mathbf{x}_i - \mathbf{x}_{k(i)}|)\chi_{\mathcal{B}_\delta}(\mathbf{x}_{k(i)}^\perp/r)|f|^2\Big] \\ \times \prod_{k=1}^n b_r(\mathbf{x}_k^\perp)^2 \mathrm{d}\mathbf{x}_k \ ,\end{aligned} \tag{8.42}$$

where $\partial_j = \mathrm{d}/\mathrm{d}z_j$, and $\nabla^\perp$ denotes the gradient in $\perp$-direction. We now investigate the last term in (8.42). Consider, for fixed $z_1, \ldots, z_n$, the expression

$$\sum_{i=1}^n \int \Big[\varepsilon|\nabla_i^\perp f|^2 + a'U(|\mathbf{x}_i - \mathbf{x}_{k(i)}|)\chi_{\mathcal{B}_\delta}(\mathbf{x}_{k(i)}^\perp/r)|f|^2\Big] \prod_{k=1}^n b_r(\mathbf{x}_k^\perp)^2 \mathrm{d}\mathbf{x}_k^\perp \ . \tag{8.43}$$

To estimate this term from below, we use Temple's inequality, as in Sect. 2.2. Let $\widetilde{e}^\perp$ denote the gap above zero in the spectrum of $-\Delta^\perp + V^\perp - e^\perp$, i.e., the lowest non-zero eigenvalue. By scaling, $\widetilde{e}^\perp/r^2$ is the gap in the spectrum of $-\Delta^\perp + V_r^\perp - e^\perp/r^2$. Note that under the transformation $\phi \mapsto b_r^{-1}\phi$ this latter operator is unitarily equivalent to $\nabla^{\perp *} \cdot \nabla^\perp$ as an operator on $L^2(\mathbb{R}^2, b_r(\mathbf{x}^\perp)^2 \mathrm{d}\mathbf{x}^\perp)$, as considered in (8.43). Hence also this operator has $\widetilde{e}^\perp/r2$ as its energy gap. Denoting

$$\langle U^k \rangle = \int \left(\sum_{i=1}^n U(|\mathbf{x}_i - \mathbf{x}_{k(i)}|)\chi_{\mathcal{B}_\delta}(\mathbf{x}_{k(i)}^\perp/r) \right)^k \prod_{k=1}^n b_r(\mathbf{x}_k^\perp)^2 \mathrm{d}\mathbf{x}_k^\perp \ , \tag{8.44}$$

Temple's inequality implies

$$(8.43) \geq |F|^2 a' \langle U \rangle \left(1 - a' \frac{\langle U^2 \rangle}{\langle U \rangle} \frac{1}{\varepsilon \widetilde{e}^\perp / r^2 - a' \langle U \rangle} \right) \ . \tag{8.45}$$

Now, using (2.30) and Schwarz's inequality, $\langle U^2 \rangle \leq 3n(R^3 - R_0^3)^{-1}\langle U \rangle$, and

$$\langle U \rangle \leq n(n-1) \frac{\|b\|_4^4}{r^2} \frac{3\pi R^2}{R^3 - R_0^3} \ . \tag{8.46}$$

Therefore

$$(8.45) \geq |F|^2 a'' \langle U \rangle \ , \tag{8.47}$$

where we put all the error terms into the modified coupling constant a''. It remains to derive a lower bound on $\langle U \rangle$. Let

$$d(z - z') = \int_{\mathbb{R}^4} b_r(\mathbf{x}^\perp)^2 b_r(\mathbf{y}^\perp)^2 U(|\mathbf{x} - \mathbf{y}|)\chi_{\mathcal{B}_\delta}(\mathbf{y}^\perp/r) \mathrm{d}\mathbf{x}^\perp \mathrm{d}\mathbf{y}^\perp \ . \tag{8.48}$$

Note that $d(z)=0$ if $|z|\geq R$. An estimate similar to (2.36) gives

$$\langle U\rangle \geq \sum_{i\neq j} d(z_i-z_j)\left(1-(n-2)\frac{\pi R^2}{r^2}\|b\|_\infty^2\right) . \tag{8.49}$$

Note that, for an appropriate choice of R, d is close to a δ-function with the desired coefficient. To make the connection with the δ-function, we can use a bit of the kinetic energy saved in (8.42) to obtain

$$\begin{aligned}\int & \left[\frac{\varepsilon}{n-1}|\partial_i F|^2 + a''' d(z_i-z_j)|F|^2\right] \mathrm{d}z_i \\ & \geq \tfrac{1}{2} g' \max_{|z_i-z_j|\leq R} |F|^2 \chi_{[R,\ell-R]}(z_j)\left(1-\left(\frac{2(n-1)}{\varepsilon}g'R\right)^{1/2}\right) . \end{aligned}\tag{8.50}$$

Putting all the previous estimates together, we arrive at

$$\begin{aligned}\langle\Psi|H|\Psi\rangle - \frac{ne^\perp}{r^2} \geq & \sum_{i=1}^n \int \left[(1-\varepsilon)|\partial_i F|^2 \chi_{\min_k |z_i-z_k|\geq R}(z_i)\right] \prod_{k=1}^n \mathrm{d}z_k \\ & + \sum_{i\neq j} \tfrac{1}{2} g'' \int \max_{|z_i-z_j|\leq R} |F|^2 \chi_{[R,\ell-R]}(z_j) \prod_{k,\,k\neq i} \mathrm{d}z_k \end{aligned}\tag{8.51}$$

for an appropriate coupling constant g'' that contains all the error terms. Now assume that $(n+1)R<\ell$. Given an F with $\int |F|^2 \mathrm{d}z_1\cdots \mathrm{d}z_n = 1$, define, for $0\leq z_1\leq z_2\leq\cdots\leq z_n\leq \ell-(n+1)R$,

$$\psi(z_1,\ldots,z_n) = F(z_1+R, z_2+2R, z_3+3R,\ldots,z_n+nR) , \tag{8.52}$$

and extend the function to all of $[0,\ell-(n+1)R]^n$ by symmetry. A simple calculation shows that

$$\begin{aligned}(8.51) \geq \langle\psi|H'|\psi\rangle & \geq (1-\varepsilon)E_{\mathrm{N}}^{\mathrm{1D}}(n,\ell-(n+1)R,g'')\langle\psi|\psi\rangle \\ & \geq (1-\varepsilon)E_{\mathrm{N}}^{\mathrm{1D}}(n,\ell,g'')\langle\psi|\psi\rangle , \end{aligned}\tag{8.53}$$

where H' is the Hamiltonian (8.3) with a factor $(1-\varepsilon)$ in front of the kinetic energy term.

It remains to estimate $\langle\psi|\psi\rangle$. Using that F is related to the true ground state Ψ by (8.41), we can estimate it in terms of the total QM energy, namely

$$\begin{aligned}\langle\psi|\psi\rangle \geq 1 & - \frac{2R}{g''}\left(E_{\mathrm{N}}^{\mathrm{QM}}(N,\ell,r,a) - \frac{ne^\perp}{r^2}\right) \\ & - 2n\frac{R}{\ell} - 4nR\left(\frac{1}{n}E_{\mathrm{N}}^{\mathrm{QM}}(n,\ell,r,a) - \frac{e^\perp}{r^2}\right)^{1/2} . \end{aligned}\tag{8.54}$$

Collecting all the error terms and choosing

$$R = r\left(\frac{a}{r}\right)^{1/4} , \quad \varepsilon = \left(\frac{a}{r}\right)^{1/8} , \quad \delta = \left(\frac{a}{r}\right)^{1/8} , \tag{8.55}$$

(8.53) and (8.54) lead to the desired lower bound. □

As already noted above, Lemma 8.3 is the key to the proof of Theorems 8.1 and 8.2. The estimates are used in each box, and the particles are distributed optimally among the boxes. For the global lower bound, superadditivity of the energy and convexity of the energy density $\rho^3 e(g/\rho)$ are used, generalizing corresponding arguments in Sect. 2. We refer to [58] for details.

9 The Charged Bose Gas, the One- and Two-Component Cases

The setting now changes abruptly. Instead of particles interacting with a short-range potential $v(|\mathbf{x}_i - \mathbf{x}_j|)$ they interact via the Coulomb potential

$$v(|\mathbf{x}_i - \mathbf{x}_j|) = |\mathbf{x}_i - \mathbf{x}_j|^{-1} \tag{9.1}$$

(in 3 dimensions). The unit of electric charge is 1 in our units.

We will here consider both the one- and two-component gases. In the one-component gas (also referred to as the one-component plasma or bosonic jellium) we consider positively charged particles confined to a box with a uniformly charged background. In the two-component gas we have particles of both positive and negative charges moving in all of space.

9.1 The One-Component Gas

In the one-component gas there are N positively charged particles in a large box Λ of volume L^3 as before, with $\rho = N/L^3$.

To offset the huge Coulomb repulsion (which would drive the particles to the walls of the box) we add a uniform negative background of precisely the same charge, namely density ρ. Our Hamiltonian is thus

$$H_N^{(1)} = \sum_{i=1}^{N} -\mu\Delta_i - V(\mathbf{x}_i) + \sum_{1\le i<j\le N} v(|\mathbf{x}_i - \mathbf{x}_j|) + C \tag{9.2}$$

with

$$V(\mathbf{x}) = \rho\int_\Lambda |\mathbf{x}-\mathbf{y}|^{-1}\mathrm{d}\mathbf{y} \qquad \text{and} \qquad C = \frac{1}{2}\rho\int_\Lambda V(\mathbf{x})\mathrm{d}\mathbf{x}\,. \tag{9.3}$$

We shall use Dirichlet boundary conditions. As before the Hamiltonian acts on symmetric wave functions in $L^2(\Lambda^N, \mathrm{d}\mathbf{x}_1\cdots\mathrm{d}\mathbf{x}_N)$.

Each particle interacts only with others and not with itself. Thus, despite the fact that the Coulomb potential is positive definite, the ground state energy E_0 can be (and is) negative (just take Ψ =const.). This time, *large* ρ is the 'weakly interacting' regime.

We know from the work in [50] that the thermodynamic limit $e_0(\rho)$ defined as in (2.2) exists. It also follows from this work that we would, in fact, get the same thermodynamic energy if we did not restrict the number of particles N, but considered the grand-canonical case where we minimize the energy over all possible particle numbers, but keeping the background charge ρ fixed.

Another way in which this problem is different from the previous one is that *perturbation theory is correct to leading order.* If one computes $(\Psi, H\Psi)$ with Ψ =const, one gets the right first order answer, namely 0. It is the next order in $1/\rho$ that is interesting, and this is *entirely* due to correlations. In 1961 Foldy [23] calculated this correlation energy according to the prescription of Bogolubov's 1947 theory. That theory was not exact for the dilute Bose gas, as we have seen, even to first order. We are now looking at *second* order, which should be even worse. Nevertheless, there was good physical intuition that this calculation should be asymptotically *exact.* Indeed it is, as proved in [60] and [82].

The Bogolubov theory states that the main contribution to the energy comes from pairing of particles into momenta $\mathbf{k}, -\mathbf{k}$ and is the bosonic analogue of the BCS theory of superconductivity which came a decade later. I.e., Ψ_0 is a sum of products of terms of the form $\exp\{i\mathbf{k}\cdot(\mathbf{x}_i - \mathbf{x}_j)\}$.

The following theorem is the main result for the one-component gas.

Theorem 9.1 (Foldy's law for the one-component gas).

$$\lim_{\rho\to\infty} \rho^{-1/4} e_0(\rho) = -\frac{2}{5}\frac{\Gamma(3/4)}{\Gamma(5/4)}\left(\frac{2}{\mu\pi}\right)^{1/4} . \tag{9.4}$$

This is the *first example* (in more than 1 dimension) in which Bogolubov's pairing theory has been rigorously validated. It has to be emphasized, however, that Foldy and Bogolubov rely on the existence of Bose–Einstein condensation. We neither make such a hypothesis nor does our result for the energy imply the existence of such condensation. As we said earlier, it is sufficient to prove condensation in small boxes of fixed size.

Incidentally, the one-dimensional example for which Bogolubov's theory is asymptotically exact to the first two orders (high density) is the repulsive delta-function Bose gas [48], for which there is no Bose–Einstein condensation.

To appreciate the $-\rho^{1/4}$ nature of (9.4), it is useful to compare it with what one would get if the bosons had infinite mass, i.e., the first term in (9.2) is dropped. Then the energy would be proportional to $-\rho^{1/3}$ as shown in [50]. Thus, the effect of quantum mechanics is to lower $\frac{1}{3}$ to $\frac{1}{4}$.

A problem somewhat related to bosonic jellium is *fermionic* jellium. Graf and Solovej [28] have proved that the first two terms are what one would expect, namely

$$e_0(\rho) = C_{\mathrm{TF}}\rho^{5/3} - C_{\mathrm{D}}\rho^{4/3} + o(\rho^{4/3}) , \tag{9.5}$$

where C_{TF} is the usual Thomas–Fermi constant and C_{D} is the usual Dirac exchange constant.

It is supposedly true, for both bosonic and fermionic particles, that there is a critical mass above which the ground state should show crystalline ordering

(Wigner crystal), but this has never been proved and it remains an intriguing open problem, even for the infinite mass case. A simple scaling shows that large mass is the same as small ρ, and is thus outside the region where a Bogolubov approximation can be expected to hold.

As for the dilute Bose gas, there are several relevant length scales in the problem of the charged Bose gas. For the dilute gas there were three scales. This time there are just two. Because of the long range nature of the Coulomb problem there is no scale corresponding to the scattering length a. One relevant length scale is again the interparticle distance $\rho^{-1/3}$. The other is the correlation length scale $\ell_{\rm cor} \sim \rho^{-1/4}$ (ignoring the dependence on μ). The order of the correlation length scale can be understood heuristically as follows. Localizing on a scale $\ell_{\rm cor}$ requires kinetic energy of the order of $\ell_{\rm cor}^{-2}$. The Coulomb potential from the particles and background on the scale $\ell_{\rm cor}$ is $(\rho\ell_{\rm cor}^3)/\ell_{\rm cor}$. Thus the kinetic energy and the Coulomb energy balance when $\ell_{\rm cor} \sim \rho^{-1/4}$. This heuristics is however much too simplified and hides the true complexity of the situation.

Note that in the high density limit $\ell_{\rm cor}$ is long compared to the interparticle distance. This is analogous to the dilute gas where the scale ℓ_c is also long compared to the interparticle distance [see (2.12)]. There is however no real analogy between the scale $\ell_{\rm cor}$ for the charged gas and the scale ℓ_c for the dilute gas. In particular, whereas $e_0(\rho)$ for the dilute gas is, up to a constant, of the same order as the kinetic energy $\sim \mu\ell_c^{-2}$ we have for the charged gas that $e_0(\rho) \not\sim \ell_{\rm cor}^{-2} = \rho^{1/2}$. The reason for this difference is that on average only a small fraction of the particles in the charged gas actually correlate.

9.2 The Two-Component Gas

Now we consider N particles with charges ± 1. The Hamiltonian is thus

$$H_N^{(2)} = \sum_{i=1}^{N} -\mu\Delta_i + \sum_{1\le i<j\le N} \frac{e_i e_j}{|\mathbf{x}_i - \mathbf{x}_j|} \,. \tag{9.6}$$

This time we are interested in $E_0^{(2)}(N)$ the ground state energy of $H_N^{(2)}$ minimized over all possible combination of charges $e_i = \pm 1$, i.e., we do not necessarily assume that the minimum occurs for the neutral case. Restricting to the neutral case would however not change the result we give below.

An equivalent formulation is to say that $E_0^{(2)}(N)$ is the ground state energy of the Hamiltonian acting on all wave functions of space and charge, i.e., functions in $L^2\left((\mathbb{R}^3 \times \{-1,1\})^N\right)$. As mentioned in the introduction, and explained in the beginning of the proof of Thm. 2.2, for the calculation of the ground state energy we may as usual restrict to symmetric functions in this Hilbert space.

For the two-component gas there is no thermodynamic limit. In fact, Dyson [18] proved that $E_0^{(2)}(N)$ was at least as negative as $-(\text{const})N^{7/5}$ as $N \to \infty$.

Thus, thermodynamic stability (i.e., a linear lower bound) fails for this gas. Years later, a lower bound of this $-N^{7/5}$ form was finally established in [12], thereby proving that this law is correct.

The connection of this $-N^{7/5}$ law with the jellium $-\rho^{1/4}$ law (for which a corresponding lower bound was also given in [12]) was pointed out by Dyson [18] in the following way. Assuming the correctness of the $-\rho^{1/4}$ law, one can treat the 2-component gas by treating each component as a background for the other. What should the density be? If the gas has a radius L and if it has N bosons then $\rho = NL^{-3}$. However, the extra kinetic energy needed to compress the gas to this radius is NL^{-2}. The total energy is then $NL^{-2} - N\rho^{1/4}$, and minimizing this with respect to L gives $L \sim N^{-1/5}$ and leads to the $-N^{7/5}$ law. The correlation length scale is now $\ell_{\text{cor}} \sim \rho^{-1/4} \sim N^{-2/5}$.

In [18] Dyson conjectured an exact asymptotic expression for $E_0^{(2)}(N)$ for large N. That this asymptotics, as formulated in the next theorem, is indeed correct is proved in [61] and [82].

Theorem 9.2 (Dyson's law for the two-component gas).

$$\lim_{N\to\infty} \frac{E_0^{(2)}(N)}{N^{7/5}} = \inf\left\{ \mu \int_{\mathbb{R}^3} |\nabla \Phi|^2 - I_0 \int_{\mathbb{R}^3} \Phi^{5/2} \,\middle|\, 0 \le \Phi,\ \int_{\mathbb{R}^3} \Phi^2 = 1 \right\}, \tag{9.7}$$

where I_0 is the constant from Foldy's law:

$$I_0 = \frac{2}{5} \frac{\Gamma(3/4)}{\Gamma(5/4)} \left(\frac{2}{\mu\pi} \right)^{1/4} . \tag{9.8}$$

This asymptotics can be understood as a mean field theory for the gas density, very much like the Gross–Pitaevskii functional for dilute trapped gases, where the local energy described by Foldy's law should be balanced by the kinetic energy of the gas density. Thus if we let the gas density be given by ϕ^2 then the "mean field" energy should be

$$\mu \int_{\mathbb{R}^3} |\nabla \phi|^2 - I_0 \int_{\mathbb{R}^3} \phi^{5/2} . \tag{9.9}$$

Here $\int \phi^2 = N$. If we now define $\Phi(\mathbf{x}) = N^{-8/5}\phi(N^{-1/5}\mathbf{x})$ we see that $\int \Phi^2 = 1$ and that the above energy is

$$N^{7/5} \left(\mu \int_{\mathbb{R}^3} |\nabla \Phi|^2 - I_0 \int_{\mathbb{R}^3} \Phi^{5/2} \right) . \tag{9.10}$$

It may be somewhat surprising that it is exactly the same constant I_0 that appears in both the one- and two-component cases. The reason that there are no extra factors to account for the difference between one and two components is, as we shall see below, a simple consequence of Bogolubov's method. The origin of this equivalence, while clear mathematically, does not appear to have a simple physical interpretation.

9.3 The Bogolubov Approximation

In this section we shall briefly explain the Bogolubov approximation and how it is applied in the case of the charged Bose gas. The Bogolubov method relies on the exact diagonalization of a Hamiltonian, which is quadratic in creation and annihilation operators. For the charged Bose gas one only needs a very simple case of the general diagonalization procedure. On the other hand, the operators that appear are not exact creation and annihilation operators. A slightly more general formulation is needed.

Theorem 9.3 (Simple case of Bogolubov's method). *Assume that $b_{\pm,\pm}$ are four (possibly unbounded) commuting operators satisfying the operator inequality*

$$\left[b_{\tau,e}, b^*_{\tau,e}\right] \leq 1 \quad \textit{for all } e, \tau = \pm \, . \tag{9.11}$$

Then for all real numbers $\mathcal{A}, \mathcal{B}_+, \mathcal{B}_- \geq 0$ we have

$$\begin{aligned}
&\mathcal{A} \sum_{\tau,e=\pm 1} b^*_{\tau,e} b_{\tau,e} \\
&\quad + \sum_{e,e'=\pm 1} \sqrt{\mathcal{B}_e \mathcal{B}_{e'}}\, e e' (b^*_{+,e} b_{+,e'} + b^*_{-,e} b_{-,e'} + b^*_{+,e} b^*_{-,e'} + b_{+,e} b_{-,e'}) \\
&\qquad \geq -(\mathcal{A} + \mathcal{B}_+ + \mathcal{B}_-) + \sqrt{(\mathcal{A} + \mathcal{B}_+ + \mathcal{B}_-)^2 - (\mathcal{B}_+ + \mathcal{B}_-)^2} \, .
\end{aligned} \tag{9.12}$$

If $b_{\pm,\pm}$ are four annihilation operators then the lower bound is sharp.

Proof. Let us introduce

$$d^*_\pm = (\mathcal{B}_+ + \mathcal{B}_-)^{-1/2} (\mathcal{B}_+^{1/2} b^*_{\pm,+} - \mathcal{B}_-^{1/2} b^*_{\pm,-}) \, , \tag{9.13}$$

and

$$c^*_\pm = (\mathcal{B}_+ + \mathcal{B}_-)^{-1/2} (\mathcal{B}_-^{1/2} b^*_{\pm,+} + \mathcal{B}_+^{1/2} b^*_{\pm,-}) \, . \tag{9.14}$$

Then these operators satisfy

$$[d_+, d^*_+] \leq 1, \quad [d_-, d^*_-] \leq 1 \, . \tag{9.15}$$

The operator that we want to estimate from below may be rewritten as

$$\begin{aligned}
&\mathcal{A}(d^*_+ d_+ + d^*_- d_- + c^*_+ c_+ + c^*_- c_-) \\
&\qquad + (\mathcal{B}_+ + \mathcal{B}_-) \left(d^*_+ d_+ + d^*_- d_- + d^*_+ d^*_- + d_+ d_-\right) \, .
\end{aligned} \tag{9.16}$$

We may now complete the squares to write this as

$$\begin{aligned}
&\mathcal{A}(c^*_+ c_+ + c^*_- c_-) + D(d^*_+ + \lambda d_-)(d^*_+ + \lambda d_-)^* \\
&\qquad + D(d^*_- + \lambda d_+)(d^*_- + \lambda d_+)^* - D\lambda^2([d_+, d^*_+] + [d_-, d^*_-])
\end{aligned} \tag{9.17}$$

if

$$D(1+\lambda^2) = \mathcal{A} + \mathcal{B}_+ + \mathcal{B}_-, \quad 2D\lambda = \mathcal{B}_+ + \mathcal{B}_- \ . \tag{9.18}$$

We choose the solution

$$\lambda = 1 + \frac{\mathcal{A}}{\mathcal{B}_+ + \mathcal{B}_-} - \sqrt{\left(1 + \frac{\mathcal{A}}{(\mathcal{B}_+ + \mathcal{B}_-)}\right)^2 - 1} \ . \tag{9.19}$$

Hence

$$D\lambda^2 = \tfrac{1}{2}\left(\mathcal{A} + \mathcal{B}_+ + \mathcal{B}_- - \sqrt{(\mathcal{A} + \mathcal{B}_+ + \mathcal{B}_-)^2 - (\mathcal{B}_+ + \mathcal{B}_-)^2}\right) \ . \tag{9.20}$$

□

In the theorem above one could of course also have included linear terms in $b_{\tau,e}$ in the Hamiltonian. In the technical proofs in [60, 61] the Bogolubov diagonalization with linear terms is indeed being used to control certain error terms. Here we shall not discuss the technical details of the proofs. We have therefore stated the theorem in the simplest form in which we shall need it to derive the leading contribution.

In our applications to the charged Bose gas the operators $b_{\pm,e}$ will correspond to the annihilation of particles with charge $e = \pm$ and momenta $\pm\mathbf{k}$ for some $\mathbf{k} \in \mathbb{R}^3$. Thus, only equal and opposite momenta couple. In a translation invariant case this would be a simple consequence of momentum conservation. The one-component gas is not translation invariant, in our formulation. The two-component gas is translation invariant, but it is natural to break translation invariance by going into the center of mass frame. In both cases it is only in some approximate sense that equal and opposite momenta couple.

In the case of the one-component gas we only need particles of one sign. In this case we use the above theorem with $b_{\pm,-} = 0$ and $\mathcal{B}_- = 0$.

We note that the lower bounds in Theorem 9.3 for the one- and two-component gases are the same except for the replacement of $\mathcal{B}_+$ in the one-component case by $\mathcal{B}_+ + \mathcal{B}_-$ in the two-component case. In the application to the two-component gas $\mathcal{B}_+$ and $\mathcal{B}_-$ will be proportional to the particle densities for respectively the positive or negatively charged particles. For the one-component gas $\mathcal{B}_+$ is proportional to the background density.

The Bogolubov diagonalization method cannot be immediately applied to the operators $H_N^{(1)}$ or $H_N^{(2)}$ since these operators are *not* quadratic in creation and annihilation operators. In fact, they are quartic. They have the general form

$$\sum_{\alpha,\beta} t_{\alpha\beta} a_\alpha^* a_\beta + \tfrac{1}{2} \sum_{\alpha,\beta,\mu,\nu} w_{\alpha\beta\mu\nu} a_\alpha^* a_\beta^* a_\nu a_\mu \ , \tag{9.21}$$

with

$$t_{\alpha\beta} = \langle\alpha|T|\beta\rangle, \qquad w_{\alpha\beta\mu\nu} = \langle\alpha\beta|W|\mu\nu\rangle \ , \tag{9.22}$$

where T is the one-body part of the Hamiltonian and W is the two-body-part of the Hamiltonian.

The main step in Bogolubov's approximation is now to assume Bose–Einstein condensation, i.e., that almost all particles are in the same one-particle state. In case of the two-component gas this means that almost half the particles are positively charged and in the same one-particle state as almost all the other half of negatively charged particles. We denote this condensate state by the index $\alpha = 0$ in the sums above. Based on the assumption of condensation Bogolubov now argues that one may ignore all terms in the quartic Hamiltonian above which contain 3 or 4 non-zero indices and at the same time replace all creation and annihilation operators of the condensate by their expectation values. The result is a quadratic Hamiltonian (including linear terms) in the creation and annihilation with non-zero index. This Hamiltonian is of course not particle number preserving, reflecting the simple fact that particles may be created out of the condensate or annihilated into the condensate.

In Sect. 9.5 below it is explained how to construct trial wave functions for the one- and two-component charged gases whose expectations agree essentially with the prescription in the Bogolubov approximation. The details are to appear in [82]. This will imply upper bounds on the energies corresponding to the asymptotic forms given in Theorems 9.1 and 9.2.

In [60, 61] it is proved how to make the steps in the Bogolubov approximation rigorous as lower bounds. The main difficulty is to control the degree of condensation. As already explained it is not necessary to prove condensation in the strong sense described above. We shall only prove condensation in small boxes. Put differently, we shall not conclude that most particles are in the same one-particle state, but rather prove that most particles occupy one-particle states that look the same on short scales, i.e., that vary slowly. Here the short scale is the correlation length scale ℓ_{cor}.

9.4 The Rigorous Lower Bounds

As already mentioned we must localize into small boxes of some fixed size ℓ. This time we must require $\ell_{\text{cor}} \ll \ell$. For the one-component gas this choice is made only in order to control the degree of condensation. For the two-component gas it is required both to control the order of condensation, and also to make a local constant density approximation. The reason we can control the degree of condensation in a small box is that the localized kinetic energy has a gap above the lowest energy state. In fact, the gap is of order ℓ^{-2}. Thus if we require that ℓ is such that $N\ell^{-2}$ is much greater than the energy we may conclude that most particles are in the lowest eigenvalue state for the localized kinetic energy. We shall always choose the localized kinetic energy in such a way that the lowest eigenstate, and hence the condensate, is simply a constant function.

Localizing the Interaction

In contrast to the dilute gas the long range Coulomb potential prevents us from simply ignoring the interaction between the small boxes. To overcome this problem we use a sliding technique first introduced in [12].

Theorem 9.4 (Controlling interactions by sliding). *Let χ be a smooth approximation to the characteristic function of the unit cube centered at the origin. For $\ell > 0$ and $\mathbf{z} \in \mathbb{R}^3$ let $\chi_{\mathbf{z}}(\mathbf{x}) = \chi((\mathbf{x}-\mathbf{z})/\ell)$. There exists an $\omega > 0$ depending on χ (in such a way that it tends to infinity as χ approximates the characteristic function) such that*

$$\sum_{1\le i<j\le N} \frac{e_i e_j}{|\mathbf{x}_i - \mathbf{x}_j|} \ge \left(\int \chi^2\right)^{-1} \int_{\mathbb{R}^3} \sum_{1\le i<j\le N} e_i e_j w_{\ell\mathbf{z}}(\mathbf{x}_i, \mathbf{x}_j) \mathrm{d}\mathbf{z} - \frac{N\omega}{2\ell}\,, \tag{9.23}$$

for all $\mathbf{x}_1, \ldots \in \mathbb{R}^3$ and $e_1, \ldots = \pm 1$, where

$$w_{\mathbf{z}}(\mathbf{x}, \mathbf{y}) = \chi_{\mathbf{z}}(\mathbf{x}) Y_{\omega/\ell}(\mathbf{x}-\mathbf{y}) \chi_{\mathbf{z}}(\mathbf{y}) \tag{9.24}$$

with $Y_\mu(\mathbf{x}) = |\mathbf{x}|^{-1} \exp(-\mu|\mathbf{x}|)$ being the Yukawa potential.

The significance of this result is that the two-body potential $w_{\mathbf{z}}$ is localized to the cube of size ℓ centered at $\ell\mathbf{z}$. The lower bound above is thus an integral over localized interactions sliding around with the integration parameter.

We have stated the sliding estimate in the form relevant to the two-component problem. There is an equivalent version for the one-component gas, where the sum of the particle-particle, particle-background, and background-background interactions may be bounded below by corresponding localized interactions.

Since $\ell \gg \ell_{\mathrm{cor}}$ the error in the sliding estimate is much smaller than $\omega N/\ell_{\mathrm{cor}}$, which for both the one and two-component gases is of order ω times the order of the energy. Thus, since ℓ is much bigger than ℓ_{cor}, we have room to let ω be very large, i.e., χ is close to the characteristic function.

Localizing the Kinetic Energy

Having described the technique to control the interaction between localized regions we turn next to the *localization of the kinetic energy.*

For the two-component gas this is done in two steps. As already mentioned it is natural to break the translation invariance of the two-component gas. We do this by localizing the system into a box of size $L' \gg N^{-1/5}$ (which as we saw is the expected size of the gas) as follows. By a partition of unity we can divide space into boxes of this size paying a localization error due to the kinetic energy of order $NL'^{-2} \ll N^{7/5}$. We control the interaction between these boxes using the sliding technique.

We may now argue, as follows, that the energy is smallest if all the particles are in just one box. For simplicity we give this argument for the case of two boxes. Suppose the two boxes have respective wave functions ψ and $\widetilde{\psi}$. The total energy of these two non-interacting boxes is $E + \widetilde{E}$. Now put all the particles in one box with the trial function $\Psi = \psi\widetilde{\psi}$. The fact that this function is not bosonic (i.e., it is not symmetric with respect to all the variables) is irrelevant because the true bosonic ground state energy is never greater than that of any trial state (Perron–Frobenius Theorem). The energy of Ψ is

$$E + \widetilde{E} + \iint \rho_\psi(\mathbf{x})|\mathbf{x} - \mathbf{y}|^{-1}\rho_{\widetilde{\psi}}(\mathbf{y})\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y} \ , \tag{9.25}$$

where ρ_ψ and $\rho_{\widetilde{\psi}}$ are the respective *charge* densities of the states ψ and $\widetilde{\psi}$. We claim that the last Coulomb term can be made non-positive. How? If it is positive then we simply change the state $\widetilde{\psi}$ by interchanging positive and negative charges (only in $\widetilde{\psi}$ and not in ψ). The reader is reminded that we have not constrained the number of positive and negative particles but only their sum. This change in $\widetilde{\psi}$ reverses the relative charge of the states ψ and $\widetilde{\psi}$ so, by symmetry the energies E and $\widetilde{E}$ do not change, whereas the Coulomb interaction changes sign.

The localization into smaller cubes of size ℓ can however not be done by a crude partition of unity localization. Indeed, this would cost a localization error of order $N\ell^{-2}$, which as explained is required to be of much greater order than the energy.

For the one-component charged gas we may instead use a Neumann localization of the kinetic energy, as for the dilute Bose gas. If we denote by $\Delta_\ell^{(\mathbf{z})}$ the Neumann Laplacian for the cube of size ℓ centered at $\mathbf{z}$ we may, in the spirit of the sliding estimate, write the Neumann localization Laplacian in all of $\mathbb{R}^3$ as

$$-\Delta = \int -\Delta_\ell^{(\ell\mathbf{z})}\mathrm{d}\mathbf{z} \ . \tag{9.26}$$

In order to write the localized kinetic energy in the same form as the localized interaction we must introduce the smooth localization χ as in Theorem 9.4. This can be achieved by ignoring the low momentum part of the kinetic energy.

More precisely, there exist $\varepsilon(\chi)$ and $s(\chi)$ such that $\varepsilon(\chi) \to 0$ and $s(\chi) \to 0$ as χ approaches the characteristic function of the unit cube and such that (see Lemma 6.1 in [60])

$$-\Delta_\ell^{(\mathbf{z})} \geq (1 - \varepsilon(\chi))\mathcal{P}_\mathbf{z}\chi_\mathbf{z}(\mathbf{x})F_{\ell s(\chi)}(-\Delta)\chi_\mathbf{z}(\mathbf{x})\mathcal{P}_\mathbf{z} \tag{9.27}$$

where $\mathcal{P}_\mathbf{z}$ denotes the projection orthogonal to constants in the cube of size ℓ centered at z and

$$F_s(u) = \frac{u^2}{u + s^{-2}} \ . \tag{9.28}$$

For $u \ll s^{-2}$ we have that $F_s(u) \ll u$. Hence the effect of F in the operator estimate above is to ignore the low momentum part of the Laplacian.

For the two-component gas one cannot use the Neumann localization as for the one-component gas. Using a Neumann localization ignores the kinetic energy corresponding to long range variations in the wave function and one would not get the kinetic energy term $\int \mu|\nabla\Phi|^2$ in (9.7). This is the essential difference between the one- and two-component cases. This problem is solved in [61] where a new kinetic energy localization technique is developed. The idea is again to separate the high and low momentum part of the kinetic energy. The high momentum part is then localized as before, whereas the low momentum part is used to connect the localized regions by a term corresponding to a discrete Laplacian. (For details and the proof the reader is referred to [61].)

Theorem 9.5 (A many body kinetic energy localization). *Let $\chi_{\mathbf{z}}$, $\mathcal{P}_{\mathbf{z}}$ and F_s be as above. There exist $\varepsilon(\chi)$ and $s(\chi)$ such that $\varepsilon(\chi)\to 0$ and $s(\chi)\to 0$ as χ approaches the characteristic function of the unit cube and such that for all normalized symmetric wave functions Ψ in $L^2((\mathbb{R}^3\times\{-1,1\})^N)$ and all $\Omega\subset\mathbb{R}^3$ we have*

$$\begin{aligned}(1+\varepsilon(\chi))\left(\Psi,\sum_{i=1}^N -\Delta_i\Psi\right) \geq \int_\Omega \Big[&(\Psi,\mathcal{P}_{\ell\mathbf{z}}\chi_{\ell\mathbf{z}}(\mathbf{x})F_{\ell s(\chi)}(-\Delta)\chi_{\ell\mathbf{z}(\mathbf{x})}\mathcal{P}_{\ell\mathbf{z}}\Psi)\\ &+\tfrac12\ell^{-2}\sum_{\substack{\mathbf{y}\in\mathbb{Z}^3\\|\mathbf{y}|=1}}(S_\Psi(\ell(\mathbf{z}+\mathbf{y}))-S_\Psi(\ell\mathbf{z}))^2\Big]\mathrm{d}\mathbf{z}\\ &-\mathrm{const.}\,\ell^{-2}\mathrm{Vol}(\Omega)\ ,\end{aligned} \tag{9.29}$$

where

$$S_\Psi(\mathbf{z})=\sqrt{\left(\Psi,(a_{0+}^*(\mathbf{z})a_{0+}(\mathbf{z})+a_{0-}^*(\mathbf{z})a_{0-}(\mathbf{z}))\Psi\right)+1}-1 \tag{9.30}$$

with $a_{0\pm}(z)$ being the annihilation of a particle of charge $\pm$ in the state given by the normalized characteristic function of the cube of size ℓ centered at $\mathbf{z}$.

The first term in the kinetic energy localization in this theorem is the same as in (9.27). The second term gives rise to a discrete Laplacian for the function $S_\Psi(\ell\mathbf{z})$, which is essentially the number of condensate particles in the cube of size ℓ centered at $\ell\mathbf{z}$. Since we will eventually conclude that most particles are in the condensate this term will after approximating the discrete Laplacian by the continuum Laplacian lead to the term $\int\mu|\nabla\phi|^2$ in (9.9). We shall not discuss this any further here.

When we apply this theorem to the two-component gas the set $\ell\Omega$ will be the box of size L' discussed above. Hence the error term $\ell^{-2}\mathrm{Vol}(\Omega)$ will be of order $L'^3/\ell^{-5}\ll(N^{2/5}\ell)^{-5}(N^{1/5}L')^3N^{7/5}$. Thus since $\ell\gg N^{-2/5}$ we may still choose $L'\gg N^{-1/5}$, as required, and have this error term be lower order than $N^{7/5}$.

Controlling the Degree of Condensation

After now having localized the problem into smaller cubes we are ready to control the degree of condensation. We recall that the condensate state is the constant function in each cube. Let us denote by $\widehat{n}_{\mathbf{z}}$ the number of excited (i.e., non-condensed particles) in the box of size ℓ centered at $\mathbf{z}$. Thus for the two-component gas $\widehat{n}_{\mathbf{z}} + a_{0+}^*(\mathbf{z})a_{0+}(\mathbf{z}) + a_{0-}^*(\mathbf{z})a_{0-}(\mathbf{z})$ is the total number of particles in the box and a similar expression gives the particle number for the one-component gas.

As discussed above we can use the fact that the kinetic energy localized to a small box has a gap above its lowest eigenvalue to control the number of excited particles. Actually, this will show that the expectation $(\Psi, \widehat{n}_{\mathbf{z}}\Psi)$ is much smaller than the total number of particles in the box for any state Ψ with negative energy expectation.

One needs, however, also a good bound on $(\Psi, \widehat{n}_{\mathbf{z}}^2\Psi)$ to control the Coulomb interaction of the non-condensed particles. This is more difficult. In [60] this is not achieved directly through a bound on $(\Psi, \widehat{n}_{\mathbf{z}}\Psi)$ in the ground state. Rather it is proved that one may change the ground state without changing its energy very much, so that it only contains values of $\widehat{n}_{\mathbf{z}}$ localized close to $(\Psi, \widehat{n}_{\mathbf{z}}\Psi)$. The following theorem gives this very general localization technique. Its proof can be found in [60].

Theorem 9.6 (Localizing large matrices). *Suppose that $\mathcal{A}$ is an $N+1 \times N+1$ Hermitean matrix and let $\mathcal{A}^k$, with $k = 0, 1, ..., N$, denote the matrix consisting of the k^{th} supra- and infra-diagonal of $\mathcal{A}$. Let $\psi \in \mathbf{C}^{N+1}$ be a normalized vector and set $d_k = (\psi, \mathcal{A}^k\psi)$ and $\lambda = (\psi, \mathcal{A}\psi) = \sum_{k=0}^{N} d_k$. ($\psi$ need not be an eigenvector of $\mathcal{A}$.)*

Choose some positive integer $M \le N+1$. Then, with M fixed, there is some $n \in [0, N+1-M]$ and some normalized vector $\phi \in \mathbf{C}^{N+1}$ with the property that $\phi_j = 0$ unless $n+1 \le j \le n+M$ (i.e., ϕ has length M) and such that

$$(\phi, \mathcal{A}\phi) \le \lambda + \frac{C}{M^2}\sum_{k=1}^{M-1} k^2|d_k| + C\sum_{k=M}^{N}|d_k| \,, \tag{9.31}$$

where $C > 0$ is a universal constant. (Note that the first sum starts with $k = 1$.)

To use this theorem we start with a ground state (or approximate ground state) Ψ to the many body problem. We then consider the projections of Ψ onto the eigenspaces of $\widehat{n}_{\mathbf{z}}$. Since the possible eigenvalues run from 0 to N these projections span an at most $N+1$ dimensional space.

We use the above theorem with $\mathcal{A}$ being the many body Hamiltonian restricted to this $N+1$ dimensional subspace. Since the Hamiltonian can change the number of excited particles by at most two we see that d_k vanishes for $k \ge 3$. We shall not here discuss the estimates on d_1 and d_2 (see [60, 61]). The conclusion is that we may, without changing the energy expectation of

Ψ too much, assume that the values of $\widehat{n}_{\mathbf{z}}$ run in an interval of length much smaller than the total number of particles. We would like to conclude that this interval is close to zero. This follows from the fact that any wave function with energy expectation close to the minimum must have an expected number of excited particles much smaller than the total number of particles.

The Quadratic Hamiltonian

Using our control on the degree of condensation it is now possible to estimate all unwanted terms in the Hamiltonian, i.e., terms that contain 3 or more creation or annihilation operators corresponding to excited (non-condensate) states. The proof which is a rather complicated bootstrapping argument is more or less the same for the one- and two-component gases. The result, in fact, shows that we can ignore other terms too. In fact if we go back to the general form (9.21) of the Hamiltonian it turns out that we can control all quartic terms except the ones with the coefficients:

$$w_{\alpha\beta 00},\ w_{00\alpha\beta},\ w_{\alpha 00\beta},\ \text{and } w_{0\alpha\beta 0}\ . \tag{9.32}$$

To be more precise, let u_α, $\alpha = 1, \ldots$ be an orthonormal basis of real functions for the subspace of functions on the cube of size ℓ centered at $\mathbf{z}$ orthogonal to constants, i.e, with vanishing average in the cube. We shall now omit the subscript $\mathbf{z}$ and let $a_{0\pm}$ be the annihilation of a particle of charge ± 1 in the normalized constant function in the cube (i.e., in the condensate). Let $a_{\alpha\pm}$ with $\alpha \neq 0$ be the annihilation operator for a particle of charge ± 1 in the state u_α. We can then show that the main contribution to the localized energy of the two-component gas comes from the Hamiltonian

$$\begin{aligned} H_{\text{local}} = &\sum_{\substack{\alpha,\beta=1\\ e=\pm 1}}^{\infty} t_{\alpha\beta} a^*_{\alpha e} a_{\beta e} \\ &+ \frac{1}{2} \sum_{\substack{\alpha,\beta=1\\ e,e'=\pm 1}} ee' w_{\alpha\beta} (2 a^*_{0e} a^*_{\alpha e'} a_{0e'} a_{\beta e} + a^*_{0e} a^*_{0e'} a_{\alpha e'} a_{\beta e} + a^*_{\alpha e} a^*_{\beta e'} a_{0e'} a_{0e})\ , \end{aligned} \tag{9.33}$$

where

$$t_{\alpha\beta} = \mu(u_\alpha, \mathcal{P}_{\mathbf{z}} \chi_{\mathbf{z}}(\mathbf{x}) F_{\ell s(\chi)}(-\Delta) \chi_{\mathbf{z}}(\mathbf{x}) \mathcal{P}_{\mathbf{z}} u_\beta) \tag{9.34}$$

and

$$w_{\alpha\beta} = \ell^{-3} \iint u_\alpha(\mathbf{x}) \chi_{\mathbf{z}}(\mathbf{x}) Y_{\omega/\ell}(\mathbf{x}-\mathbf{y}) \chi_{\mathbf{z}}(\mathbf{y}) u_\beta(\mathbf{x}) \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y}\ . \tag{9.35}$$

In H_{local} we have ignored all error terms and hence also $\varepsilon(\chi) \approx 0$ and $\int \chi^2 \approx 1$.

In the case of the one-component gas we get exactly the same local Hamiltonian, except that we have only one type of particles, i.e, we may set $a_{\alpha -} = 0$ above.

Let $\nu_\pm = \sum_{\alpha=0}^{\infty} a_{\alpha\pm}^* a_{\alpha\pm}$ be the total number of particles in the box with charge ± 1. For $\mathbf{k} \in \mathbb{R}^3$ we let $\chi_{\mathbf{k},\mathbf{z}}(\mathbf{x}) = \chi_{\mathbf{z}}(\mathbf{x}) e^{i\mathbf{k}\cdot\mathbf{x}}$. We then introduce the operators

$$b_{\mathbf{k}\pm} = (\ell^3 \nu_\pm)^{-1/2} a_\pm(\mathcal{P}_{\mathbf{z}} \chi_{\mathbf{k},\mathbf{z}}) a_{0\pm}^* \ , \tag{9.36}$$

where $a_\pm(\mathcal{P}_{\mathbf{z}}\chi_{\mathbf{k},\mathbf{z}}) = \sum_{\alpha=1}^{\infty} (\chi_{\mathbf{k},\mathbf{z}}, u_\alpha) a_{\alpha\pm}$ annihilates a particle in the state $\chi_{\mathbf{k},\mathbf{z}}$ with charge ± 1. It is then clear that the operators $b_{\mathbf{k}\pm}$ all commute and a straightforward calculation shows that

$$[b_{\mathbf{k}\pm}, b_{\mathbf{k}\pm}^*] \le (\ell^3 \nu_\pm)^{-1} \|\mathcal{P}_{\mathbf{z}} \chi_{\mathbf{z}}\|^2 a_{0\pm}^* a_{0\pm} \le 1 \ . \tag{9.37}$$

If we observe that

$$\begin{aligned} \sum_{\substack{\alpha,\beta=1 \\ e=\pm 1}}^{\infty} t_{\alpha\beta} a_{\alpha e}^* a_{\beta e} &= (2\pi)^{-3} \int \mu F_{\ell s(\chi)}(\mathbf{k}^2) \sum_{e=\pm} a_e(\mathcal{P}_{\mathbf{z}}\chi_{\mathbf{k},\mathbf{z}})^* a_e(\mathcal{P}_{\mathbf{z}}\chi_{\mathbf{k},\mathbf{z}}) \mathrm{d}\mathbf{k} \\ &\ge (2\pi)^{-3} \ell^3 \int \mu F_{\ell s(\chi)}(\mathbf{k}^2) \sum_{e=\pm} b_{\mathbf{k}e}^* b_{\mathbf{k}e} \ , \end{aligned} \tag{9.38}$$

we see that

$$\begin{aligned} H_{\mathrm{local}} \ge \tfrac{1}{2}(2\pi)^{-3} \int \Big[&\mu \ell^3 F_{\ell s(\chi)}(\mathbf{k}^2) \sum_{e=\pm} (b_{\mathbf{k}e}^* b_{\mathbf{k}e} + b_{-\mathbf{k}e}^* b_{-\mathbf{k}e}) \\ &+ \sum_{ee'=\pm} \widehat{Y}_{\omega/\ell}(\mathbf{k}) \sqrt{\nu_e \nu_{e'}}\, ee' (b_{\mathbf{k}e}^* b_{\mathbf{k},e'} + b_{-\mathbf{k}e}^* b_{-\mathbf{k},e'} + b_{\mathbf{k}e}^* b_{-\mathbf{k},e'}^* + b_{-\mathbf{k}e} b_{\mathbf{k},e'}) \Big] \mathrm{d}\mathbf{k} \\ &- \sum_{\alpha\beta=1} w_{\alpha\beta} (a_{\alpha+}^* a_{\beta+} + a_{\alpha-}^* a_{\beta-}) \end{aligned} \tag{9.39}$$

The last term comes from commuting $a_{0\pm}^* a_{0\pm}$ to $a_{0\pm} a_{0\pm}^*$. It is easy to see that this last term is a bounded operator with norm bounded by

$$\text{const.}\, (\nu_+ + \nu_-) \ell^{-3} \|\widehat{Y}_{\omega/\ell}\|_\infty \le \text{const.}\, \omega^{-2} (\nu_+ + \nu_-) \ell^{-1} \ . \tag{9.40}$$

When summing over all boxes we see that the last term above gives a contribution bounded by $\text{const.}\, \omega^{-2} N \ell^{-1} = \omega^{-2} (N^{2/5}\ell)^{-1} N^{7/5}$ which is lower order than the energy.

The integrand in the lower bound on H_{local} is precisely an operator of the form treated in the Bogolubov method Theorem 9.3. Thus up to negligible errors we see that the operator H_{local} is bounded below by

$$\tfrac{1}{2}(2\pi)^{-3} \int -(\mathcal{A}(\mathbf{k}) + \mathcal{B}(\mathbf{k})) + \sqrt{(\mathcal{A}(\mathbf{k}) + \mathcal{B}(\mathbf{k}))^2 - \mathcal{B}(\mathbf{k})^2}\, \mathrm{d}\mathbf{k} \ , \tag{9.41}$$

where

$$\mathcal{A}(\mathbf{k}) = \mu \ell^3 F_{\ell s(\chi)}(\mathbf{k}^2) \quad \text{and} \quad \mathcal{B}(\mathbf{k}) = \nu \widehat{Y}_{\omega/\ell}(\mathbf{k}) \tag{9.42}$$

with $\nu = \nu_+ + \nu_-$ being the total number of particles in the small box. A fairly simple analysis of the above integral shows that we may to leading order replace $\mathcal{A}$ by $\mu\ell^3\mathbf{k}^2$ and $\mathcal{B}(\mathbf{k})$ by $4\pi\nu|\mathbf{k}|^{-2}$, i.e., we may ignore the cut-offs. The final conclusion is that the local energy is given to leading order by

$$\frac{-1}{2(2\pi)^3}\int 4\pi\nu|\mathbf{k}|^{-2}+\mu\ell^3|\mathbf{k}|^2-\sqrt{(4\pi\nu|\mathbf{k}|^{-2}+\mu\ell^3|\mathbf{k}|^2)^2-(4\pi\nu|\mathbf{k}|^{-2})^2}\,\mathrm{d}\mathbf{k}$$
$$=-2^{1/2}\pi^{-3/4}\nu\left(\frac{\nu}{\mu\ell^3}\right)^{1/4}\int_0^\infty 1+x^4-x^2(2+x^4)^{1/2}\,\mathrm{d}x\,. \quad (9.43)$$

If we finally use that

$$\int_0^\infty 1+x^4-x^2(2+x^4)^{1/2}\,\mathrm{d}x=\frac{2^{3/4}\sqrt{\pi}\Gamma(3/4)}{5\Gamma(5/4)} \quad (9.44)$$

we see that the local energy to leading order is $-I_0\nu(\nu/\ell^3)^{1/4}$. For the one-component gas we should set $\nu=\rho\ell^3$ and for the two-component gas we should set $\nu=\phi^2\ell^3$ (see (9.9)). After replacing the sum over boxes by an integral and at the same time replace the discrete Laplacian by a continuum Laplacian, as described above, we arrive at asymptotic lower bounds as in Theorems 9.1 and 9.2.

There is one issue that we have not discussed at all and which played an important role in the treatment of the dilute gas. How do we know the number of particles in each of the small cubes? For the dilute gas a superadditivity argument was used to show that there was an equipartition of particles among the smaller boxes. Such an argument cannot be used for the charged gas. For the one-component gas one simply minimizes the energy over all possible particle numbers in each little box. It turns out that charge neutrality is essentially required for the energy to be minimized. Since the background charge in each box is fixed this fixes the particle number.

For the two-component there is a-priori nothing that fixes the particle number in each box. More precisely, if we ignored the kinetic energy between the small boxes it would be energetically favorable to put all particles in one small box. It is the kinetic energy between boxes, i.e., the discrete Laplacian term in Theorem 9.5, that prevents this from happening. Thus we could in principle again minimize over all particle numbers and hope to prove the correct particle number dependence (i.e., Foldy's law) in each small box. This is essentially what is done except that boxes with very many or very few particles must be treated somewhat differently from the "good" boxes. In the "bad" boxes we do not prove Foldy's law, but only weaker estimates that are adequate for the argument.

9.5 The Rigorous Upper Bounds

The Upper Bound for the Two-component Gas

To prove an upper bound on the energy $E_0^{(2)}(N)$ of the form given in Dyson's formula Theorem 9.2 we shall construct a trial function from the prescription in the Bogolubov approximation. We shall use as an input a minimizer Φ for the variational problem on the right side of (9.7). That minimizers exist can be easily seen using spherical decreasing rearrangements. It is however not important that a minimizer exists. An approximate minimizer would also do for the argument given here. Define $\phi_0(\mathbf{x}) = N^{3/10}\Phi(N^{1/5}\mathbf{x})$. Then again $\int \phi_0^2 = 1$. In terms of the unscaled function ϕ in (9.9), $\phi_0(\mathbf{x}) = N^{-1}\phi(\mathbf{x})$.

Let ϕ_α, $\alpha = 1, \ldots$ be an orthonormal family of real functions all orthogonal to ϕ_0. We choose these functions below.

We follow Dyson [18] and choose a trial function which does not have a specified particle number, i.e., a state in the bosonic Fock space.

As our trial many-body wave function we now choose

$$\begin{aligned}\Psi &= \exp\left(-\lambda_0^2 + \lambda_0 a_{0+}^* + \lambda_0 a_{0-}^*\right) \\ &\quad\times \prod_{\alpha\neq 0}(1-\lambda_\alpha^2)^{1/4}\exp\Big(-\sum_{e,e'=\pm 1}\sum_{\alpha\neq 0}\frac{\lambda_\alpha}{4}ee' a_{\alpha,e}^* a_{\alpha,e'}^*\Big)\,|0\rangle\ ,\end{aligned} \tag{9.45}$$

where $a_{\alpha,e}^*$ is the creation of a particle of charge $e = \pm 1$ in the state ϕ_α, $|0\rangle$ is the vacuum state, and the coefficients $\lambda_0, \lambda_1, \ldots$ will be chosen below satisfying $0 < \lambda_\alpha < 1$ for $\alpha \neq 0$.

It is straightforward to check that Ψ is a normalized function.

Dyson used a very similar trial state in [18], but in his case the exponent was a purely quadratic expression in creation operators, whereas the one used here is only quadratic in the creation operators $a_{\alpha e}^*$, with $\alpha \neq 0$ and linear in $a_{0\pm}^*$. As a consequence our state will be more sharply localized around the mean of the particle number.

In fact, the above trial state is precisely what is suggested by the Bogolubov approximation. To see this note that one has

$$(a_{0\pm} - \lambda_0)\Psi = 0, \qquad \text{and} \qquad \left(a_{\alpha+}^* - a_{\alpha-}^* + \lambda_\alpha(a_{\alpha+} - a_{\alpha-})\right)\Psi = 0 \tag{9.46}$$

for all $\alpha \neq 0$. Thus the creation operators for the condensed states can be replaced by their expectation values and an adequate quadratic expression in the non-condensed creation and annihilation operators is minimized.

Consider now the operator

$$\gamma = \sum_{\alpha=1}^{\infty}\frac{\lambda_\alpha^2}{1-\lambda_\alpha^2}|\phi_\alpha\rangle\langle\phi_\alpha|\ . \tag{9.47}$$

A straightforward calculation of the energy expectation in the state Ψ gives that

$$\left(\Psi, \sum_{N=0}^{\infty} H_N^{(2)} \Psi\right) = 2\lambda_0^2 \mu \int (\nabla\phi_0)^2 + \mathrm{Tr}\,(-\mu\Delta\gamma) \\ + 2\lambda_0^2 \mathrm{Tr}\left(\mathcal{K}\left(\gamma - \sqrt{\gamma(\gamma+1)}\right)\right) , \tag{9.48}$$

where $\mathcal{K}$ is the operator with integral kernel

$$\mathcal{K}(\mathbf{x}, \mathbf{y}) = \phi_0(\mathbf{x})|\mathbf{x} - \mathbf{y}|^{-1}\phi_0(\mathbf{y}) . \tag{9.49}$$

Moreover, the expected particle number in the state Ψ is $2\lambda_0^2 + \mathrm{Tr}(\gamma)$. In order for Ψ to be well defined by the formula (9.45) we must require this expectation to be finite.

Instead of making explicit choices for the individual functions ϕ_α and the coefficients λ_α, $\alpha \neq 0$ we may equivalently choose the operator γ. In defining γ we use the method of coherent states. Let χ be a non-negative real and smooth function supported in the unit ball in $\mathbb{R}^3$, with $\int \chi^2 = 1$. Let as before $N^{-2/5} \ll \ell \ll N^{-1/5}$ and define $\chi_\ell(\mathbf{x}) = \ell^{-3/2}\chi(\mathbf{x}/\ell)$. We choose

$$\gamma = (2\pi)^{-3} \int_{\mathbb{R}^3\times\mathbb{R}^3} f(\mathbf{u}, |\mathbf{p}|)\mathcal{P}_{\phi_0}^{\perp} |\theta_{\mathbf{u},\mathbf{p}}\rangle\langle\theta_{\mathbf{u},\mathbf{p}}| \mathcal{P}_{\phi_0}^{\perp} \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{p} \tag{9.50}$$

where $\mathcal{P}_{\phi_0}^{\perp}$ is the projection orthogonal to ϕ_0,

$$\theta_{\mathbf{u},\mathbf{p}}(x) = \exp(i\mathbf{p}\cdot\mathbf{x})\chi_\ell(\mathbf{x} - \mathbf{u}) , \tag{9.51}$$

and

$$f(\mathbf{u}, |\mathbf{p}|) = \frac{1}{2}\left(\frac{\mathbf{p}^4 + 16\pi\lambda_0^2\mu^{-1}\phi_0(\mathbf{u})^2}{\mathbf{p}^2\left(\mathbf{p}^4 + 32\pi\lambda_0^2\mu^{-1}\phi_0(\mathbf{u})^2\right)^{1/2}} - 1\right) . \tag{9.52}$$

We note that γ is a positive trace class operator, $\gamma\phi_0 = 0$, and that all eigenfunctions of γ may be chosen real. These are precisely the requirements needed in order for γ to define the orthonormal family ϕ_α and the coefficients λ_α for $\alpha \neq 0$.

We use the following version of the Berezin–Lieb inequality [5, 46]. Assume that $\xi(t)$ is an *operator* concave function of $\mathbb{R}_+ \cup \{0\}$ with $\xi(0) \geq 0$. Then if Y is a positive semi-definite operator we have

$$\mathrm{Tr}\,(Y\xi(\gamma)) \geq (2\pi)^{-3} \int \xi(f(\mathbf{u}, |\mathbf{p}|))\left(\theta_{\mathbf{u},\mathbf{p}}, \mathcal{P}_{\phi_0}^{\perp} Y \mathcal{P}_{\phi_0}^{\perp}\theta_{\mathbf{u},\mathbf{p}}\right) \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{p} . \tag{9.53}$$

We use this for the function $\xi(t) = \sqrt{t(t+1)}$. Of course, if ξ is the identity function then (9.53) is an identity. If $Y = I$ then (9.53) holds for all concave ξ with $\xi(0) \geq 0$.

Proving an upper bound on the energy expectation (9.48) is thus reduced to the calculations of explicit integrals. After estimating these integrals one arrives at the leading contribution (for large λ_0)

$$
\begin{aligned}
2\lambda_0^2\mu \int (\nabla\phi_0)^2 + \iint \left(\mu\mathbf{p}^2 + 2\lambda_0^2\phi_0(\mathbf{u})^2\frac{4\pi}{\mathbf{p}^2}\right) f(\mathbf{u},|\mathbf{p}|) \\
- \frac{4\pi}{\mathbf{p}^2} 2\lambda_0^2\phi_0(\mathbf{u})^2\sqrt{f(\mathbf{u},|\mathbf{p}|)(f(\mathbf{u},|\mathbf{p}|)+1)}\,\mathrm{d}\mathbf{p}\mathrm{d}\mathbf{u} \\
= 2\lambda_0^2\mu \int (\nabla\phi_0)^2 - I_0 \int (2\lambda_0^2)^{5/4}\phi_0^{5/2}\,, \quad (9.54)
\end{aligned}
$$

where I_0 is as in Theorem 9.2.

If we choose $\lambda_0 = \sqrt{N/2}$ we get after a simple rescaling that the energy above is $N^{7/5}$ times the right side of (9.7) (recall that Φ was chosen as the minimizer). We also note that the expected number of particles is

$$
2\lambda_0^2 + \mathrm{Tr}(\gamma) = N + O(N^{3/5})\,, \qquad (9.55)
$$

as $N \to \infty$.

The only remaining problem is to show how a similar energy could be achieved with a wave function with a fixed number of particles N, i.e., how to show that we really have an upper bound on $E_0^{(2)}(N)$. We indicate this fairly simple argument here.

We construct a trial function Ψ' as above, but with an expected particle number N' chosen appropriately close to, but slightly smaller than N. More precisely, N' will be smaller than N by an appropriate lower order correction. It is easy to see then that the mean deviation of the particle number distribution in the state Ψ' is lower order than N. In fact, it is of order $\sqrt{N'} \sim \sqrt{N}$. Using that we have a good lower bound on the energy $E_0^{(2)}(n)$ for all n and that Ψ' is sharply localized around its mean particle number, we may, without changing the energy expectation significantly, replace Ψ' by a normalized wave function Ψ that only has particle numbers less than N. Since the function $n \mapsto E_0^{(2)}(n)$ is a decreasing function we see that the energy expectation in the state Ψ is, in fact, an upper bound to $E_0^{(2)}(N)$.

The Upper Bound for the One-component Gas

The upper bound for the one-component gas is proved in a very similar way as for the two-component gas. We shall simply indicate the main differences here. We will again choose a trial state without a fixed particle number, i.e., a grand canonical trial state. Since we know that the one-component gas has a thermodynamic limit and that there is equivalence of ensembles [50], it makes no difference whether we choose a canonical or grand-canonical trial state.

For the state ϕ_0 we now choose a normalized function with compact support in Λ, that is constant on the set $\{x \in \Lambda \mid \mathrm{dist}(x, \partial\Lambda) > r\}$. We shall choose $r > 0$ to go to zero as $L \to \infty$. Let us also choose the constant n such that $n\phi_0^2 = \rho$ on the set where ϕ_0 is constant. Then $n \approx \rho L^3$.

Let again ϕ_α, $\alpha = 1, \dots$ be an orthonormal family of real functions orthogonal to ϕ_0. As our trial state we choose, this time,

$$\Psi = \prod_{\alpha\neq 0}(1-\lambda_\alpha^2)^{1/4}\exp\Big(-\lambda_0^2/2+\lambda_0 a_0^* - \sum_{\alpha\neq 0}\frac{\lambda_\alpha}{2}a_\alpha^* a_\alpha^*\Big)\,|0\rangle\ , \qquad (9.56)$$

where a_α^* is the creation of a particle in the state ϕ_α. We will choose Ψ implicitly by choosing the operator γ defined as in (9.47).

This time we obtain

$$\begin{aligned}\Big(\Psi,\sum_{N=0}^{\infty}H_N^{(1)}\Psi\Big) &= \lambda_0^2\mu\int(\nabla\phi_0)^2 \\ &+ \tfrac12\iint\frac{|\gamma(\mathbf{x},\mathbf{y})|^2}{|\mathbf{x}-\mathbf{y}|}\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y} + \tfrac12\iint\frac{|\sqrt{\gamma(\gamma+1)}(\mathbf{x},\mathbf{y})|^2}{|\mathbf{x}-\mathbf{y}|}\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y} \\ &+ \tfrac12\iint_{\Lambda\times\Lambda}\frac{\left(\rho-\rho_\gamma(\mathbf{x})-\lambda_0^2\phi_0(\mathbf{x})^2\right)\left(\rho-\rho_\gamma(\mathbf{y})-\lambda_0^2\phi_0(\mathbf{y})^2\right)}{|\mathbf{x}-\mathbf{y}|}\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y} \\ &+ \mathrm{Tr}\,(-\mu\Delta\gamma)+\lambda_0^2\mathrm{Tr}\left(\mathcal{K}\left(\gamma-\sqrt{\gamma(\gamma+1)}\right)\right)\ ,\end{aligned} \qquad (9.57)$$

where $\rho_\gamma(\mathbf{x})=\gamma(\mathbf{x},\mathbf{x})$ and $\mathcal{K}$ is again given as in (9.49). We must show that we can make choices such that the first four terms on the right side above are lower order than the energy, and can therefore be neglected.

We choose

$$\gamma=\gamma_\varepsilon=(2\pi)^{-3}\int_{|p|>\varepsilon\rho^{1/4}} f(|\mathbf{p}|)\mathcal{P}_{\phi_0}^{\perp}|\theta_{\mathbf{p}}\rangle\langle\theta_{\mathbf{p}}|\mathcal{P}_{\phi_0}^{\perp}\mathrm{d}\mathbf{p}\ , \qquad (9.58)$$

where $\varepsilon>0$ is a parameter which we will let tend to 0 at the end of the calculation. Here $\mathcal{P}_{\phi_0}^{\perp}$ as before is the projection orthogonal to ϕ_0 and this time

$$f(|\mathbf{p}|)=\frac12\left(\frac{\mathbf{p}^4+8\pi\mu^{-1}\rho}{\mathbf{p}^2\left(\mathbf{p}^4+16\pi\mu^{-1}\rho\right)^{1/2}}-1\right) \qquad (9.59)$$

and

$$\theta_{\mathbf{p}}(x)=\sqrt{n\rho^{-1}}\exp(i\mathbf{p}\cdot\mathbf{x})\phi_0(\mathbf{x})\ . \qquad (9.60)$$

Note that $n\rho^{-1}\phi_0(\mathbf{x})^2$ is 1 on most of Λ. We then again have the Berezin–Lieb inequality as before. We also find that

$$\begin{aligned}\rho_\gamma(\mathbf{x}) &= (2\pi)^{-3}\int_{|p|>\varepsilon\rho^{1/4}} f(|\mathbf{p}|)\mathrm{d}\mathbf{p}\,n\rho^{-1}\phi_0(\mathbf{x})^2\left(1+O(\varepsilon^{-1}\rho^{-1/4}L^{-1})\right) \\ &= A_\varepsilon(\rho/\mu)^{3/4}n\rho^{-1}\phi_0(\mathbf{x})^2\left(1+O(\varepsilon^{-1}\rho^{-1/4}L^{-1})\right)\ ,\end{aligned} \qquad (9.61)$$

where A_ε is an explicit function of ε. We now choose λ_0 such that $\lambda_0^2 = n(1-A_\varepsilon\rho^{-1/4}\mu^{-3/4})$, i.e., such that

$$\lambda_0^2\phi_0^2(\mathbf{x})+\rho_\gamma(\mathbf{x})=n\phi_0(\mathbf{x})^2(1+O(\varepsilon^{-1}\rho^{-1/2}L^{-1}))\approx\rho\ . \qquad (9.62)$$

It is easy to see that the first term in (9.57) is of order $\rho L^3(rL)^{-1}$ and the fourth term in (9.57) is of order $\rho L^3(\varepsilon^{-2}+\rho r^2)$. We may choose r, depending on L, in such a way that after dividing by ρL^3 and letting $L\to\infty$ only the error ε^{-2} remains. This allows choosing $\varepsilon \ll \rho^{-1/8}$.

To estimate the second term in (9.57) we use Hardy's inequality to deduce

$$\iint \frac{|\gamma(\mathbf{x},\mathbf{y})|^2}{|\mathbf{x}-\mathbf{y}|}\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y} \le 2(\mathrm{Tr}\,\gamma^2)^{1/2}\mathrm{Tr}\,(-\Delta\gamma^2)^{1/2}\,, \tag{9.63}$$

and these terms can be easily estimated using the Berezin–Lieb inequality in the direction opposite from before, since we are interested now in an upper bound. The third term in (9.57) is controlled in exactly the same way as the second term. We are then left with the last two terms in (9.57). They are treated in exactly the same way as for the two-component gas again using the Berezin–Lieb inequality.

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Meromorphic Inner Functions, Toeplitz Kernels and the Uncertainty Principle

N. Makarov[1]* and A. Poltoratski[2]**

[1] California Institute of Technology, Department of Mathematics, Pasadena, CA 91125, USA makarov@its.caltech.edu
[2] Texas A&M University, Department of Mathematics, College Station, TX 77843, USA alexeip@math.tamu.edu

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1 Introduction

This paper touches upon several traditional topics of 1D linear complex analysis including distribution of zeros of entire functions, completeness problem for complex exponentials and for other families of special functions, some problems of spectral theory of selfadjoint differential operators. Their common feature is the close relation to the theory of complex Fourier transform of compactly supported measures or, more generally, Fourier–Weyl–Titchmarsh transforms associated with selfadjoint differential operators with compact resolvent.

The last part of the title is a reference to the monograph [19], which contains a large collection of results that could be described by the (informal) statement: "it is impossible for a non-zero function and its Fourier transform to be simultaneously very small." For example, if a function is supported

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on a small interval, then the set of zeros of its Fourier transform has to be sparse. Another example: a small amount of information about the potential of a Schrödinger operator requires a large amount of information about the spectral measure to determine the operator uniquely.

Our goal is to present a unified approach to certain problems of this type. The method is based on the reduction (complete or partial) to the injectivity problem for Toeplitz operators, which makes it possible to use the full strength of the theory of Hardy–Nevanlinna classes and Hilbert transform rather than rely on the standard techniques of the theory of entire function (Jensen type formulae, canonical products, Phragmen–Lindelöf principle). We have been able to reinterpret various classical results (often with shorter proofs and stronger conclusions) in a way that allows further generalizations. We explain the reason for such generalizations (and their nature) below. We begin by briefly describing the background.

1.1 Complex Exponentials, Paley–Wiener Spaces, and Cartwright Functions

If $a > 0$ and $\Lambda \subset \mathbb{C}$, then by the very definition of the classical Fourier transform,

$$f(t) \mapsto \hat{f}(z) = \int \mathrm{e}^{\mathrm{i}zt} f(t)\mathrm{d}t \,, \tag{1}$$

the family of exponential functions $\mathcal{E}_\Lambda = \left\{\mathrm{e}^{\mathrm{i}\lambda t} :\ \lambda \in \Lambda\right\}$ is not complete in $L^2(-a,a)$ if and only if there is a non-trivial function F from the *Paley–Wiener space*

$$\mathrm{PW}_a = \{\hat{f} :\ f \in L^2(-a,a)\} \,,$$

such that $F = 0$ on Λ. According to Paley–Wiener's theorem, see [33], PW_a can be characterized as the space of entire functions which have exponential type at most a and are square summable on the real line $\mathbb{R}$.

The *Cartwright class* $\mathrm{Cart_a}$, $a \geq 0$, consists of entire functions F of exponential type at most a satisfying a weaker integrability condition on $\mathbb{R}$:

$$\log^+ |F| \in L^1(\mathbb{R}, \Pi) \,, \qquad \mathrm{d}\Pi(t) := \frac{\mathrm{d}t}{1+t^2} \,.$$

Cartwright functions are considered in detail in the monographs [29], [6], [28], [12], [25], [19]. The following *Krein's theorem* [26] is important for the purpose of this discussion: an entire function is Cartwright if and only if it belongs to the Nevanlinna class in the lower and in the upper halfplanes. In a sense, Paley–Wiener spaces are to Cartwright spaces as the Hardy space $\mathcal{H}^2$ is to the Smirnov–Nevanlinna class $\mathcal{N}^+$. The precise meaning of this analogy, which is only true up to an arbitrarily small gap in the exponential type, is a part of the deep Beurling–Malliavin theory [4], [5].

The growth limitations (exponential type and integrability conditions on $\mathbb{R}$) on Paley–Wiener and Cartwright functions carry with them severe limitations on the distribution of zeros. This is a central theme of the classical theory of entire functions, and numerous results have been obtained in the study of the relation between the growth and zeros. Let us mention some principle facts. For a set Λ we denote by $N(R)$ the number of points $\lambda \in \Lambda$ satisfying $|\lambda| < R$, and by $N_\pm(R)$ the number of points λ, $|\lambda| < R$, such that $\Re\lambda > 0$ and $\Re\lambda < 0$ respectively.

Density and symmetry of zeros. If F is a non-trivial Cartwright function and Λ is the set of all zeros, then the limits

$$\lim_{R\to\infty} \frac{N_\pm(R)}{R}$$

exist, are finite and equal. Moreover, there exists a finite limit

$$\text{v.p.} \sum \frac{1}{\lambda} \equiv \lim_{R\to\infty} \sum_{|\lambda|<R} \frac{1}{\lambda} \,.$$

See, e.g., [28], [25].

Levinson's completeness theorem. If F is a non-trivial function in PW_a and $F = 0$ on Λ (so $\mathcal{E}_\Lambda$ is not complete in $L^2[-a,a]$), then

$$\lim_{R\to\infty} \left[\int_1^R \frac{N(t)}{t} \mathrm{d}t - \frac{2a}{\pi} R + \frac{1}{2} \log R \right] = -\infty \,.$$

Some other sufficient conditions for completeness are known, as well as some necessary conditions, see [38], [41]. On the other hand, finding an effective general metric criterion does not seem to be realistically possible.

Beurling–Malliavin theory. The most interesting and deep result in the completeness problem is the metric characterization of the "radius of completeness",

$$R(\Lambda) = \sup\{a : \ \mathcal{E}_\Lambda \quad \text{complete in} \quad L^2(-a,a)\} \,,$$

obtained in [4]–[5]. Beurling and Malliavin described $R(\Lambda)$ as a certain "density" $d_{\mathrm{BM}}(\Lambda)$, which is defined in a non-trivial but completely computable way. We recall the definition of $d_{\mathrm{BM}}(\Lambda)$ and discuss the Beurling–Malliavin theory in the last part of the paper.

Let us now explain how the completeness problem can be restated in terms of Toeplitz kernels.

1.2 Model Spaces and Toeplitz Operators

By the Paley–Wiener theorem, the Fourier transform (1) identifies $L^2(0,\infty)$ with the Hardy space $\mathcal{H}^2$ in the upper halfplane $\mathbb{C}_+$, and therefore it identifies $L^2(\pm a,\infty)$ with $S^{\pm a}H^2$. Here and *throughout* the paper, S denotes the singular inner function

$$S(z) = \mathrm{e}^{\mathrm{i}z} \,.$$

It follows that the Paley–Wiener spaces have the following representation:

$$\mathrm{PW}_a = S^{-a}\left[\mathcal{H}^2 \ominus S^{2a}\mathcal{H}^2\right] .$$

The subspace $\mathcal{H}^2 \ominus S^{2a}\mathcal{H}^2$ is the so called model space of the inner function S^{2a}. More generally, one defines model spaces

$$K_\Theta \equiv K[\Theta] = \mathcal{H}^2 \ominus \Theta\mathcal{H}^2$$

for all inner functions Θ in $\mathbb{C}_+$; these spaces play an important role in the modern function theory and also in the spectral theory, see [34], [27]. Strictly speaking, the elements of K_Θ are functions in $\mathbb{C}_+$ but if Θ is a meromorphic inner function, then every element has a meromorphic continuation to the whole complex plane. In particular, the completeness problem for exponentials is exactly the problem of describing the uniqueness sets of the model spaces $K[S^{2a}]$.

If $U \in L^\infty(\mathbb{R})$, then the *Toeplitz operator* with *symbol* U is the map

$$T_U : \mathcal{H}^2 \to \mathcal{H}^2 , \qquad F \mapsto P_+(UF) ,$$

where P_+ is the orthogonal projection in $L^2(\mathbb{R})$ onto $\mathcal{H}^2$. A one line argument shows that $\Lambda \subset \mathbb{C}_+$ is a uniqueness set of K_Θ if and only if the kernel of the Toeplitz operator T_U is trivial, where

$$U = \bar{\Theta}B_\Lambda , \qquad B_\Lambda \quad \text{Blaschke product} .$$

(There is a similar statement for general sets $\Lambda \subset \mathbb{C}$, see Sect. 4.1.)

The *injectivity problem* – to characterize symbols U such that $\ker\, T_U = 0$ – is of interest in its own right as part of the spectral theory of Toeplitz operators, see [8], [35]. Compared with some other aspects of the theory such as invertibility problem, the injectivity problem has attracted relatively little attention. Let us mention the important paper [23] where the idea to use (invertibility) properties of Toeplitz operators in the study of bases of exponentials was introduced, see also [3].

We can now explain our goal more clearly. We would like to see if the classical results mentioned above could be extended to Toeplitz operators with more general symbols. More precisely, we'll be considering real-analytic symbols $U = \mathrm{e}^{\mathrm{i}\gamma}$, $\gamma \in C^\omega(\mathbb{R})$, so that infinity is the only "singularity" of the symbol. A special case (which is in fact just as general, see [9]) is the case of symbols of the form

$$U = \bar{\Theta}J ,$$

where Θ and J are meromorphic inner functions. We will show now that the injectivity problem for operators with such symbols appears as naturally as in the special case $\Theta = S^{2a}$.

1.3 Spectral Theory

Consider the Schrödinger equation

$$-\ddot{u} + qu = \lambda u \tag{2}$$

on some interval (a, b) and assume that the potential $q(t)$ is locally integrable and a is a regular point, i.e. a if finite and q is L^1 at a. Let us fix some selfadjoint boundary condition at b and consider the Weyl m–function

$$m(\lambda) = \frac{\dot{u}_\lambda(a)}{u_\lambda(a)}\,, \qquad \lambda \notin \mathbb{R}\,,$$

where $u_\lambda(t)$ is any non-trivial solution of (2) satisfying the boundary condition. We will deal only with the *compact resolvent* case, which is equivalent to saying that m extends to a meromorphic function. Then we can define the meromorphic inner function

$$\Theta = \frac{m - \mathrm{i}}{m + \mathrm{i}}\,,$$

which we call the *Weyl inner function* associated with the potential and the fixed boundary condition at b.

The transformation

$$f(t) \;\mapsto\; F(\lambda) = \int_a^b f(t) \frac{u_\lambda(t)}{\dot{u}_\lambda(a) + \mathrm{i} u_\lambda(a)}\,\mathrm{d}t \tag{3}$$

identifies $L^2(a, b)$ with the model space K_Θ in the same way as the classical Fourier transform (times S^a) identifies $L^2(-a, a)$ with $K[S^{2a}]$. This allows us to interpret the completeness problem for families of solutions $\{u_\lambda :\ \lambda \in \Lambda\}$ as a problem of uniqueness sets in the model space of Θ. Completeness problems of this type, particularly problems involving families of special functions, are well-known in the literature, see e.g. [20]. As we explained, they are equivalent to the invertibility problem for symbols $\bar{\Theta}J$, where Θ is a Weyl inner function.

Similar invertibility problems appear in connection with the uniqueness part of the inverse spectral problem. We discuss such applications in Sect. 4. Here we only mention that the results represent a rather broad generalization of such well-known facts as *Borg's two spectra theorem* [7]: two different spectra of a Schrodinger operator with compact resolvent determine the operator uniquely, and *Hochstadt–Liberman theorem* [21] that states that a regular Schrödinger operator on a finite interval is determined by its spectrum and the potential on one half of the interval. In the language of inner functions, the corresponding problems can be stated as follows.

Given a meromorphic inner function Θ and one of its factors Ψ, the problem is to decide whether this factor and the set $\{\Theta = 1\}$ determine Θ uniquely. The second problem is to describe *defining sets* of a given meromorphic inner function Φ. We say that $\Lambda \subset \mathbb{R}$ is defining if

$$\tilde{\Phi} = \Phi\,, \;\; \arg \tilde{\Phi} = \arg \Phi \text{ on } \Lambda \quad \Rightarrow \quad \tilde{\Phi} \equiv \Phi\,.$$

1.4 Content of the Paper

Section 2. *Meromorphic Inner Functions and Spectral Theory.*

2.1–2.4: We recall standard facts concerning meromorphic inner functions, their model spaces, and Weyl–Titchmarsh functions of second order selfadjoint differential operators.

2.5: We discuss the modified Fourier transform (3). In the case of regular operators, this is essentially the usual Weyl–Titchmarsh transform, but the construction is probably new in the (more interesting) singular case.

2.6–2.8: Basics of de Branges functions and associated spaces of Paley–Wiener and Cartwright type.

Section 3. *Toeplitz Kernels.*

3.1–3.4: We define the kernels and state some general (mostly known) facts. As an example, we give a Toeplitz kernel interpretation of a standard asymptotic formula for solutions of a regular Schrödinger equation.

3.5–3.6: Basic criterion for non-triviality of a Toeplitz kernel with real analytic symbol. For instance, the kernel is non-trivial in the Smirnov–Nevanlinna class if and only if the argument γ of the symbol has a representation $\gamma = -\alpha + \tilde{h}$, where $\alpha \in C^\omega$ is an increasing function and $h \in L^1_\Pi$. Though this observation is very simple (and its versions in the non-analytic case are well known), the criterion turns out to be quite workable, and the rest of the paper is mostly the study and applications of this criterion.

3.7–3.8: Kolmogorov's type criterion. This is a special case where the symbol is $\bar{H}/H$, H is an outer function, and the kernel is a priory finite dimensional. This situation is typical when we explicitly know the de Branges functions. Another useful example is the twin inner function theorem: if $\{\Theta = 1\} = \{J = 1\}$, then $\ker\ T_{\bar{\Theta}J} = 0$.

3.9–3.11: General form of Levinson's completeness theorem. We obtain a sufficient condition for triviality of a Toeplitz kernel that improves Levinson's theorem (and other similar results) even in the classical situation. The key ingredient of the proof is the Titchmarsh–Uly'anov theorem involving the so called A–integrals.

Section 4. *Some Applications.*

4.1–4.2: Completeness and minimality problem, and uniqueness sets of the model and de Branges spaces.

4.3–4.4: Distribution of zeros of functions in Cartwright–de Branges spaces. In particular, we give a new proof of the density and symmetry result mentioned in Sect. 1.1, which is based on our basic criterion and the Titchmarsh–Uly'anov theorem.

4.5–4.7: Applications to the mixed data spectral problem stated in Sect. 1.3. For the inner function version of the Hochstadt–Liberman problem we establish some necessary and some sufficient conditions in terms of Toeplitz kernels. We also give a spectral theory interpretation of these conditions indicating stronger versions of practically all known results in this area.

4.8–4.9: Remarks on defining sets of inner functions and regular Schrödinger operators.

Section 5. *Beurling–Malliavin Theory.*

5.1–5.2: Multiplier theorems. First we state a multiplier theorem for Toeplitz kernels in $\mathcal{H}^p$–spaces. Then we discuss some consequences of the Beurling–Malliavin multiplier theorem for Toeplitz kernels in the Smirnov–Nevanlinna class. We make no comments on the proof of the Beurling–Malliavin multiplier theorem itself. The presence of the Dirichlet space condition remains the most amazing feature of the theory.

5.3–5.6: Second Beurling–Malliavin and little multiplier theorems. For symbols $U = \mathrm{e}^{\mathrm{i}\gamma}$ with $\gamma' > -\mathrm{const}$, we present a complete proof of the metric criterion for (non-)triviality of a Toeplitz kernel in the Smirnov–Nevanlinna class up to a gap $S^{\pm\epsilon}$. The proof is of course not totally original but our version, we believe, is better fit for generalizations.

5.7–5.9: We discuss possible generalizations of the Beurling–Malliavin theory. We mention partial results, examples, and indicate applications in the case $\gamma'(t) > -\mathrm{const}\ |t|^a$.

2 Meromorphic Inner Functions and Spectral Theory

Function Theory in the Halfplane

2.1 Basic Notations

$\mathbb{C}_+$ is the upper half plane $\{\Re z > 0\}$. For general references concerning Hardy–Nevanlinna theory in $\mathbb{C}_+$ see [16] and [35].

We use the standard notation $\mathcal{H}^p = \mathcal{H}^p(\mathbb{C}_+)$, $0 < p \leq \infty$, for the Hardy spaces, and $\mathcal{N}^+ = \mathcal{N}^+(\mathbb{C}_+)$ for the V. I. Smirnov (or Smirnov–Nevanlinna) class in $\mathbb{C}_+$. The elements in $\mathcal{N}^+$ are ratios G/H, where $G, H \in H^\infty$ and H is an outer function. Functions in $\mathcal{N}^+$ have angular boundary values (almost everywhere) on the real line. As a general rule, we identify functions in the halfplane with their boundary values on $\mathbb{R}$. In this sense, we have

$$\mathcal{H}^p = \mathcal{N}^+ \cap L^p(\mathbb{R}) \ ,$$

and

$$F \in \mathcal{N}^+ \quad \Rightarrow \quad \log|F| \in L^1_\Pi \equiv L^1(\mathbb{R}, \Pi) \ ,$$

where Π is the Poisson measure

$$\mathrm{d}\Pi(t) = \frac{\mathrm{d}t}{1+t^2} \ .$$

If $h \in L^1_\Pi$ is a real-valued function, then its *Schwarz integral* is

$$\mathcal{S}h(z) = \frac{1}{\pi \mathrm{i}} \int \left[\frac{1}{t-z} - \frac{t}{1+t^2} \right] h(t)\mathrm{d}t \ .$$

The real and the imaginary parts of $\mathcal{S}h$ are the *Poisson* and the *conjugate Poisson integrals* of h:

$$\mathcal{S}h = \mathcal{P}h + \mathrm{i}\mathcal{Q}h \ .$$

Outer functions are functions of the form

$$H = \mathrm{e}^{\mathcal{S}h} \ , \qquad h \in L^1_\Pi \ ;$$

note that $H \in \mathcal{N}^+$ and H has modulus e^h on $\mathbb{R}$. Every function F in $\mathcal{N}^+$ has a unique factorization $F = IH$, where H is the outer function with modulus $|F|$ on $\mathbb{R}$ and I is an *inner* function, i.e. $I \in \mathcal{H}^\infty$ and $|I| = 1$ on $\mathbb{R}$.

The *Hilbert transform* of $h \in L^1_\Pi$ is the angular limit of Qh, so the outer function $\mathrm{e}^{\mathcal{S}h}$ is equal to $\mathrm{e}^{h+\mathrm{i}\tilde{h}}$ on $\mathbb{R}$. The Hilbert transform can also be defined as a singular integral:

$$\tilde{h}(x) = \frac{1}{\pi} \ \text{v.p.} \int \left[\frac{1}{x-t} + \frac{t}{1+t^2} \right] h(t)\mathrm{d}t \ .$$

For further references, we recall some properties of the Hilbert transform. If both h and $g = \tilde{h}$ are in L^1_Π, then $\tilde{g} = -h + \text{const}$, i.e.

$$\mathcal{S}\tilde{h} = -\mathrm{i}\mathcal{S}h + \mathrm{i}\mathcal{S}h(\mathrm{i}) \ .$$

If $h \in L^1_\Pi$, then $\tilde{h} \in L^{o(1,\infty)}_\Pi$ (the weak L^1 space), i.e.

$$\Pi\{|\tilde{h}| > A\} = o\left(\frac{1}{A}\right) \ , \qquad A \to \infty \ ,$$

in particular $\tilde{h} \in L^p_\Pi$ for all $p < 1$.

2.2 Meromorphic Inner Functions and Herglotz Functions

A meromorphic inner function is an inner function Θ in $\mathbb{C}_+$ which has a meromorphic extension to $\mathbb{C}$. Such a function can be characterized by parameters (a, Λ) in the canonical (Riesz–Smirnov) factorization

$$\Theta = B_\Lambda S^a \ , \tag{4}$$

where $a \geq 0$, and Λ is a discrete set (possibly with multiple points) in $\mathbb{C}_+$ satisfying the Blaschke condition

$$\sum \frac{\Im\lambda}{1+|\lambda|^2} < \infty \;;$$

B_Λ denotes the corresponding Blaschke product and $S^a(z) = \mathrm{e}^{\mathrm{i}az}$. Let us mention an obvious but important property of meromorphic inner functions:

$$\Theta = \mathrm{e}^{\mathrm{i}\theta} \quad \text{on } \mathbb{R} \;, \qquad \theta \text{ is a real analytic, increasing function.}$$

A meromorphic Herglotz function is a meromorphic function m such that

$$\Im m > 0 \text{ in } \mathbb{C}_+ \;, \qquad m(\bar{z}) = \overline{m(z)} \;.$$

One can establish a one-to-one correspondence between meromorphic inner and Herglotz functions by means of the equations

$$m = \mathrm{i}\frac{1+\Theta}{1-\Theta} \;, \qquad \Theta = \frac{m-\mathrm{i}}{m+\mathrm{i}} \;. \tag{5}$$

Meromorphic Herglotz functions (and therefore inner functions) can be described by parameters (b, c, μ) in the Herglotz representation

$$m(z) = bz + c + \mathrm{i}S\mu \;, \tag{6}$$

where $b \geq 0$, $c \in \mathbb{R}$, and μ is a positive discrete measure on $\mathbb{R}$ satisfying

$$\int \frac{\mathrm{d}\mu(t)}{1+t^2} < \infty \;.$$

It is convenient to interpret the number πb as a point mass of μ at infinity. In the case $m = m_\Theta$, see (5), we call this extended measure μ_Θ the *spectral* (or *Herglotz*) *measure* of Θ. By definition, the (point) *spectrum* of Θ is the set

$$\sigma(\Theta) = \operatorname{supp} \mu_\Theta = \{\Theta = 1\} \text{ or } \{\Theta = 1\} \cup \{\infty\} \;,$$

and by residue calculus we have

$$\mu_\Theta(t) = \frac{2\pi}{|\Theta'(t)|} \;, \qquad t \in \sigma(\Theta) \;. \tag{7}$$

The following *equivalent* conditions are necessary and sufficient for $\mu_\Theta(\infty) \neq 0$, see e.g. [36]:

$$(i) \quad \Theta - 1 \in H^2 \;; \qquad (ii) \quad \Theta(\infty) = 1 \;, \; \exists \Theta'(\infty) \;; \qquad (iii) \quad \sum \Im\lambda < \infty \;.$$

In (ii), $\Theta(\infty)$ and $\Theta'(\infty)$ mean the angular limit and angular derivative at infinity:

$$\Theta(\infty) = \lim_{y\to+\infty} \Theta(\mathrm{i}y) \ , \qquad \Theta'(\infty) = \lim_{y\to+\infty} y^2\Theta'(\mathrm{i}y)$$

and in (iii) we also require that the singular factor is trivial.

Riesz–Smirnov and Herglotz parametrizations (4)–(6) reflect two different structures – multiplicative and convex – in the set of inner functions. These structures are related in a non-trivial and intriguing way. For example, the middle point of the segment $[\Theta_1, \Theta_2]$, i.e. the inner function such that its Herglotz measure is the average of μ_{Θ_1} and μ_{Θ_2}, is the function

$$\Theta = \frac{\Theta_1 + \Theta_2 - 2\Theta_1\Theta_2}{2 - \Theta_1 - \Theta_2} \ ,$$

and we observe that

$$\Psi|\Theta_1 \ , \ \Psi|\Theta_2 \quad \Rightarrow \quad \Psi|\Theta \ ,$$

where the notation $\Psi|\Theta$ for two inner functions means that Ψ is a *factor* of Θ, i.e. Θ/Ψ is also an inner function.

2.3 Model Spaces

The $\mathcal{H}^2$–model space of an inner function Θ,

$$K_\Theta \equiv K[\Theta] = \mathcal{H}^2 \ominus \Theta\mathcal{H}^2 = \mathcal{H}^2 \cap \Theta\bar{\mathcal{H}}^2 \ ,$$

is a Hilbert space with reproducing kernel:

$$k_\lambda^\Theta(z) = \frac{1}{2\pi\mathrm{i}} \frac{1 - \overline{\Theta(\lambda)}\Theta(z)}{\bar{\lambda} - z} \ , \qquad \lambda \in \mathbb{C}_+ \ . \tag{8}$$

If Θ is meromorphic, then all elements of K_Θ are meromorphic, and one can extend (8) to all $\lambda \in \mathbb{R}$.

The monograph [34] provides a comprehensive study of model spaces. One of the important facts of the theory is the following Plancherel theorem (see Clark's paper [10] for the case of general inner functions):

Theorem 2.1. *The restriction map*

$$\mathcal{C}_\Theta : \ f \mapsto f|_{\sigma(\Theta)} \tag{9}$$

is a unitary operator $K_\Theta \to L^2(\mu_\Theta)$.

We also define the model spaces in the Smirnov class and in general Hardy spaces:

$$K_\Theta^+ = \{F \in \mathcal{N}^+ \cap C^\omega(\mathbb{R}) : \ \Theta\bar{F} \in \mathcal{N}^+\} \ ,$$

and

$$K_\Theta^p = K_\Theta^+ \cap L^p(\mathbb{R}) \ .$$

If $p \geq 1$, we can drop the requirement $F \in C^\omega(\mathbb{R})$ by Morera's theorem.

Second Order Differential Operators

2.4 Weyl Inner Functions

Meromorphic inner functions appear in the theory of second order selfadjoint differential operators with *compact* resolvent. We will only discuss the case of Schrödinger operators though similar theories exist for general canonical systems. See [32] and [30] for the basics of the spectral theory.

Let q be a real locally integrable function on (a, b). We always assume that selfadjoint operators associated with the differential operation $u \mapsto -\ddot{u} + qu$ have *compact resolvent.* We suppose that a is a *regular* point but we allow b to be infinite and/or singular. Let us fix a selfadjoint boundary condition β at b; for example, β means $u \in L^2$ at b in the limit point case. The Weyl–Titchmarsh m–function of $(q; b, \beta)$ evaluated at a,

$$m(\lambda) = m^a_{b,\beta}(\lambda) , \qquad \lambda \in \mathbb{C} ,$$

is defined by the formula

$$m(\lambda) = \frac{\dot{u}_\lambda(a)}{u_\lambda(a)} ,$$

where $u_\lambda(\cdot)$ is a non-trivial solution of the Schrödinger equation satisfying the boundary condition at b. It is well-known that m is a Herglotz function, and therefore we can define the corresponding inner function $\Theta^a_{b,\beta}$ by (5). We will call $\Theta^a_{b,\beta}$ the *Weyl* (or Weyl–Titchmarsh) *inner function* of q.

Similarly, if $b \in \mathbb{R}$ is a *regular* point and α is a selfadjoint boundary condition at $a \in [-\infty, b)$, we can consider the m–function of $(q; a, \alpha)$ evaluated at b,

$$m^b_{a,\alpha}(\lambda) = -\frac{\dot{u}_\lambda(b)}{u_\lambda(b)}$$

(mind the sign!) and define the corresponding Weyl inner function $\Theta^b_{a,\alpha}$.

Example 2.2. The Weyl inner functions of the potential $q \equiv 0$ on $[0, 1]$ with Dirichlet and, respectively, Neumann boundary conditions at $a = 0$ are

$$\Theta_D(\lambda) = \frac{\sqrt{\lambda}\cos\sqrt{\lambda} + \mathrm{i}\sin\sqrt{\lambda}}{\sqrt{\lambda}\cos\sqrt{\lambda} - \mathrm{i}\sin\sqrt{\lambda}} , \qquad \Theta_N(\lambda) = \frac{\sqrt{\lambda}\sin\sqrt{\lambda} - \mathrm{i}\cos\sqrt{\lambda}}{\sqrt{\lambda}\sin\sqrt{\lambda} + \mathrm{i}\cos\sqrt{\lambda}} . \quad (10)$$

(The m–functions are $m_D(\lambda) = -\sqrt{\lambda}\cot\sqrt{\lambda}$ and $m_N(\lambda) = \sqrt{\lambda}\tan\sqrt{\lambda}$.)

More generally, for $\nu \geq -1/2$ consider the potential

$$q(t) = \frac{\nu^2 - \frac{1}{4}}{t^2} \quad \text{on } (0, 1) ,$$

and let the boundary condition α at $a = 0$ be satisfied by the solution

$$u_\lambda(t) = \sqrt{t} J_\nu(t\sqrt{\lambda})$$

of the Schrödinger equation. For example, if $\nu = -1/2$ then $\alpha = (N)$, and if $\nu = 1/2$ then $\alpha = (D)$, and we have the limit point case if $\nu \geq 1$. J_ν is of course the standard notation for the Bessel function of order ν. Since

$$u_\lambda(1) = J_\nu(\sqrt{\lambda}) \ , \qquad \dot{u}_\lambda(1) = \frac{1}{2} J_\nu(\sqrt{\lambda}) + \sqrt{\lambda} J'_\nu(\sqrt{\lambda}) \ ,$$

the corresponding Weyl inner function is

$$\Theta_\nu(\lambda) = \frac{\sqrt{\lambda} J'_\nu(\sqrt{\lambda}) + (1/2 + \mathrm{i}) J_\nu(\sqrt{\lambda})}{\sqrt{\lambda} J'_\nu(\sqrt{\lambda}) + (1/2 - \mathrm{i}) J_\nu(\sqrt{\lambda})} \ . \tag{11}$$

In particular, we have $\Theta_{-1/2} = \Theta_N$ and $\Theta_{1/2} = \Theta_D$.

One can give many other similar examples involving special functions. We will continue to discuss Bessel inner function in Sects. 2.6 and 4.7. Our goal is to illustrate certain constructions in the singular case as opposed to the regular case, which is well presented in the literature.

2.5 Modified Fourier Transform

Let $\Theta = \Theta^a_{b,\beta}$ be the Weyl–Titchmarsh inner function of a potential q defined in the previous section. We will construct a unitary operator $L^2(a,b) \to K_\Theta$, which is a modification of the Weyl–Titchmarsh Fourier transform. We modify the usual construction so that the case of a singular endpoint b could be included.

For every $z \in \mathbb{C}$ we choose a non-trivial solution $u_z(t)$ of the Schrödinger equation satisfying the boundary condition β. (For real z such a solution exists because of the compact resolvent assumption.) If $z \in \mathbb{C}_+ \cup \mathbb{R}$, then the solution

$$w_z(t) = \frac{u_z(t)}{\dot{u}_z(a) + \mathrm{i} u_z(a)}$$

does not depend on the choice of u_z, and $w_z \in L^2(a,b)$. The transform $\mathcal{W}$ is defined as follows:

$$\mathcal{W} : \ f(t) \mapsto F(z) = \int_a^b f(t) w_z(t) \mathrm{d}t \ , \qquad (z \in \mathbb{C}_+ \cup \mathbb{R}) \ . \tag{12}$$

To state the main result we introduce the *dual reproducing kernel* of the model space K_Θ. For $\lambda \in \mathbb{C}_+ \cup \mathbb{R}$ we define

$$k^*_\lambda(z) = \frac{1}{2\pi \mathrm{i}} \frac{\Theta(z) - \Theta(\lambda)}{z - \lambda} \ , \qquad (z \in \mathbb{C}_+ \cup \mathbb{R}) \ , \tag{13}$$

so we have

$$\bar{\Theta} k^\Theta_\lambda = \overline{k^*_\lambda} \quad \text{on } \mathbb{R} \ ,$$

and $k^*_\lambda \in K_\Theta$. Note that if $\lambda \in \mathbb{R}$, then $k^*_\lambda = \text{const}\ k^\Theta_\lambda$.

Theorem 2.3. *The modified Fourier transform $\mathcal{W}$ is (up to a factor $\sqrt{\pi}$) a unitary operator $L^2(a,b) \to K_\Theta$. Furthermore, we have*

$$\mathcal{W} w_\lambda = \pi k_\lambda^* \ , \quad \mathcal{W} \bar{w}_\lambda = \pi k_\lambda \qquad (\lambda \in \mathbb{C}_+ \cup \mathbb{R}) \ . \tag{14}$$

Proof. The formulae (14) follow from the Lagrange identity

$$(z-\lambda) \int_a^b u_\lambda u_z = u_\lambda(a) \dot{u}_z(a) - \dot{u}_\lambda(a) u_z(a) \ .$$

(The Wronskian at b is zero because the two solutions satisfy the same boundary conditions.) The rest is straightforward:

$$(\bar{w}_\lambda, \bar{w}_\mu)_{L^2} = \int_a^b w_\mu \bar{w}_\lambda = \mathcal{W} \bar{w}_\lambda(\mu) = \pi k_\lambda(\mu) = \pi (k_\lambda, k_\mu)_{K_\Theta} \ ,$$

etc. □

Note that Weyl inner functions of Schrödinger operators have no point masses at infinity, so if $\Theta = \Theta^a_{b,\beta}$, then

$$\sigma(\Theta) = \sigma(q, D, \beta) \ , \qquad \sigma(-\Theta) = \sigma(q, N, \beta) \ .$$

Here $\sigma(q, D, \beta)$ means the spectrum of the Schrödinger operator with potential q, Dirichlet boundary condition at a, and boundary condition β at b. More generally, for $\alpha \in \mathbb{R}$ let α denote the following selfadjoint boundary condition at a regular endpoint a:

$$\cos \frac{\alpha}{2} u(a) + \sin \frac{\alpha}{2} \dot{u}(a) = 0 \ . \tag{15}$$

Then

$$\sigma(\mathrm{e}^{-\mathrm{i}\alpha} \Theta) = \sigma(q, \alpha, \beta) \ .$$

By definition, the spectral measure of the Schrödinger operator (q, α, β) is the Herglotz measure of the inner function $\mathrm{e}^{-\mathrm{i}\alpha}\Theta$.

Corollary 2.4. *Let $\Theta = \Theta^a_{b,\beta}$. The composition of the modified Fourier transform and the Plancherel–Clark operator* (9),

$$L^2(a,b) \xrightarrow{\mathcal{W}} K_\Theta \xrightarrow{\mathcal{C}_\Theta} L^2(\mu_\Theta) \ ,$$

is a unitary operator; it provides a spectral representation of the Schrödinger operator (q, D, β).

Entire Functions

2.6 de Branges Functions

Following [28] we say that an entire function E is of *Hermite–Biehler class* (HB) if E has no real zeros and

$$z \in \mathbb{C}_+ \quad \Rightarrow \quad |E(\bar{z})| < |E(z)| \,.$$

Every $E \in$(HB) defines a meromorphic inner function

$$\Theta_E = \frac{E^\#}{E} \,, \qquad E^\#(z) := \overline{E(\bar{z})} \,.$$

Conversely, given an inner function Θ, any $E \in$ (HB) satisfying $\Theta = \Theta_E$ is called a *de Branges function of* Θ.

It can be shown, see [12], that *every meromorphic inner function has at least one de Branges function.* In some cases one can construct de Branges functions explicitly.

Example 2.5. Let (a, b) be a finite interval and $q \in L^1(a, b)$. Given a selfadjoint boundary condition (15) at a, let $u_\lambda(t)$ denote the solution of the initial value problem

$$u_\lambda(a) = -\sin\frac{\alpha}{2} \,, \qquad \dot{u}_\lambda(a) = \cos\frac{\alpha}{2} \,. \tag{16}$$

for the Schrödinger equation. Then

$$E(\lambda) = -\dot{u}_\lambda(b) + \mathrm{i}u_\lambda(b) \tag{17}$$

is a de Branges function of the Weyl inner function $\Theta = \Theta^b_{a,\alpha}$. Indeed, we have

$$\Theta(\lambda) = \frac{-\dot{u}_\lambda(b) - \mathrm{i}u_\lambda(b)}{-\dot{u}_\lambda(b) + \mathrm{i}u_\lambda(b)} \,,$$

and the functions $\lambda \mapsto u_\lambda(b)$ and $\lambda \mapsto \dot{u}_\lambda(b)$ are entire because of the fixed initial conditions; clearly, they can not be both zero at the same point $\lambda \in \mathbb{R}$.

Example 2.6. Consider now the Bessel inner functions Θ_ν, see (11). Note that the above construction does not apply in the singular case. From the theory of Bessel's functions we know that

$$J_\nu(z) = z^\nu G_\nu(z) \,,$$

where G_ν is an even real entire function and $G_\nu(0) \neq 0$. We also introduce an even real entire function

$$F_\nu(z) = zG'_\nu(z) \,.$$

Since $zJ'_\nu = z^\nu(\nu G_\nu + F_\nu)$, we have

$$\Theta_\nu(\lambda) = \frac{F_\nu(\sqrt{\lambda}) + (1/2 + \nu + \mathrm{i})G_\nu(\sqrt{\lambda})}{F_\nu(\sqrt{\lambda}) + (1/2 + \nu - \mathrm{i})G_\nu(\sqrt{\lambda})} .$$

The function

$$E_\nu(\lambda) := F_\nu(\sqrt{\lambda}) + (1/2 + \nu - \mathrm{i})G_\nu(\sqrt{\lambda})$$

does not vanish at $\lambda = 0$ and therefore it has no zeros on $\mathbb{R}$. It follows that E_ν is a de Branges function of Θ_ν. Similar considerations work for other special functions.

Example 2.7. Some more elementary (but important) examples include the following. If $a > 0$, then $E(z) = \mathrm{e}^{-\mathrm{i}az}$ is a de Branges function of $\Theta = S^{2a}$. Polynomials with all roots in $\mathbb{C}_-$ are de Branges functions of finite Blaschke products.

2.7 Spaces of Entire Functions

We first define the *Cartwright–de Branges* space $B^+(E)$ of entire functions associated with a Hermite–Biehler function E:

$$B^+(E) = \left\{F : \ F/E, \ F^\#/E \in \mathcal{N}^+(\mathbb{C}_+)\right\} .$$

Proposition 2.8. $B^+(E) = EK^+\left[\Theta_E\right]$.

Proof. If $G \in K^+_\Theta$, then its meromorphic extension to $\mathbb{C}_-$ is equal to $H^\#/\Theta^\#$ for some $H \in \mathcal{N}^+(\mathbb{C}_+)$. Since $E = \Theta^\# E^\#$ in $\mathbb{C}_-$, the function

$$F = \begin{cases} E(z)\ G(z) & z \in \mathbb{C}_+ \ , \\ E^\#(z)H^\#(z) & z \in \mathbb{C}_- \ , \end{cases}$$

is entire and $F \in B^+(E)$. The opposite direction is similar. □

The special case $E = S^{-a}$ gives *Cartwright spaces*

$$\mathrm{Cart_a} = \mathrm{B}^+\left(\mathrm{S^{-a}}\right) = \mathrm{S^{-a}K^+}\left[\mathrm{S^{2a}}\right] , \qquad (\mathrm{a} \geq 0) .$$

Next we define the *de Branges space* associated with $E \in (HB)$, see [12]:

$$B(E) = B^+(E) \cap L^2\left(|E(x)|^{-2}\mathrm{d}x\right) = EK\left[\Theta_E\right] .$$

The special case $E = S^{-a}$ gives the *Paley–Wiener spaces*

$$\mathrm{PW}_a = B\left(S^{-a}\right) = \mathrm{Cart_a} \cap \mathrm{L^2}(\mathbb{R}) , \qquad (\mathrm{a} > 0).$$

De Branges space $B(E)$ has a natural Hilbert space structure so that the multiplication operator

$$E : \ K\left[\Theta_E\right] \to B(E)$$

is an isometry. We denote by K^E_λ, $(\lambda \in \mathbb{C})$, the reproducing kernel of $B(E)$. Theorem 2.3 has the following corollary, which is a counterpart of the Paley–Wiener theorem concerning the classical Fourier transform. Recall that $\mathcal{W}$ denotes the modified Fourier transform (12).

Corollary 2.9. *Let E be a de Branges function of the Weyl inner function $\Theta^a_{b,\beta}$ associated with a potential q on (a,b). Then the map*

$$\mathcal{F} : L^2(a,b) \to B(E) , \qquad f \mapsto E \cdot \mathcal{W} f ,$$

is a unitary operator. Furthermore, we have

$$\mathcal{F} u_\lambda = \text{const } K^E_{\bar{\lambda}} , \qquad \lambda \in \mathbb{C} ,$$

where u_λ is any non-trivial solution of the Schrödinger equation satisfying the boundary condition β.

In the *regular* case $a, b \in \mathbb{R}$ and $q \in L^1(a,b)$, the map $\mathcal{F}$ is precisely the Weyl–Titchmarsh transform

$$f \mapsto \int_a^b f(t) u_\lambda(t) \mathrm{d}t ,$$

where the solutions $u_\lambda(t)$ are normalized by initial conditions (16) and the de Branges function is given by (17).

The classical Fourier transform (1) originates from the first order self-adjoint operator $u \mapsto -\mathrm{i}u'$. Alternatively, it can be related to the Weyl–Titchmarsh transforms corresponding to $q \equiv 0$ by a general construction which we describe below, cf. [14].

2.8 Square Root Transformation

It is well-known that if m is a Herglotz function such that

$$0 < m < +\infty \quad \text{on } \mathbb{R}_- ,$$

then $m^*(\lambda) = \lambda m(\lambda^2)$ is again a Herglotz function. If $\Theta = (m - \mathrm{i})/(m + \mathrm{i})$, then the inner function corresponding to m^* is

$$\Theta^*(z) = \frac{(z+1)\Theta(z^2) + (z-1)}{(z-1)\Theta(z^2) + (z+1)}$$

We call Θ^* the square root transform of Θ. Suppose now that $E = A + \mathrm{i}B$ is a de Branges function of Θ, where A and B are real entire functions, and also suppose $B(0) \neq 0$. Then

$$E^*(z) = zA(z^2) + \mathrm{i}B(z^2)$$

is a de Branges function of Θ^*.

Example 2.10. Let $q \in L^1[0,1]$ be such that the operator $L(q, D, N) \geq 0$. Consider the function

$$m(\lambda) = \frac{u(\lambda)}{\dot{u}(\lambda)} := \frac{u_\lambda(1)}{\dot{u}_\lambda(1)} ,$$

where u_λ is the solution of the Schrödinger equation with initial conditions $u_\lambda(0) = 0$ and $\dot{u}_\lambda(0) = 1$. (In other words, m is the Herglotz function of $-\Theta^1_{0,D}$.) Then we have $E = u + \mathrm{i}\dot{u}$ and therefore

$$E^*(z) = zu(z^2) + \mathrm{i}\dot{u}(z^2) .$$

In particular, if $q \equiv 0$, then $E^*(z) = \mathrm{i}e^{-\mathrm{i}z}$, and we get the classical Paley–Wiener space.

3 Toeplitz Kernels

Some Generalities

3.1 Definition of Toeplitz Kernels

Recall that to every $U \in L^\infty(\mathbb{R})$, there corresponds the Toeplitz operator $T_U : \mathcal{H}^2 \to \mathcal{H}^2$. We need to consider only the case of *unimodular* symbols

$$U = \mathrm{e}^{\mathrm{i}\gamma} , \qquad \gamma : \mathbb{R} \to \mathbb{R} ,$$

and we will concentrate on the question whether the *Toeplitz kernel*

$$N[U] = \ker\ T_U$$

is trivial or non-trivial. The best known situation is when $\gamma \in C(\mathbb{R})$ and there exist finite limits $\gamma(\pm\infty)$. (This corresponds to the case of piecewise continuous symbols in the theory on the unit circle.) If we denote

$$\delta = \gamma(+\infty) - \gamma(-\infty) ,$$

then

$$N[U] = 0 \text{ if } \delta > -\pi , \qquad N[U] \neq 0 \text{ if } \delta < -\pi .$$

(If $\delta = -\pi$, then either case is possible.)

Along with $\mathcal{H}^2$–kernels, we define Toeplitz kernels in the Smirnov class,

$$N^+[U] = \{F \in \mathcal{N}^+ \cap L^1_{\mathrm{loc}}(\mathbb{R}) :\ \bar{U}\bar{F} \in \mathcal{N}^+\} ,$$

and in all Hardy spaces,

$$N^p[U] = N^+[U] \cap L^p(\mathbb{R}) , \qquad (0 < p \leq \infty) .$$

These definitions are oriented to studying the case where ∞ is the only “singularity” of the symbol. In particular, if Θ is a meromorphic inner function, then $N^+[\bar{\Theta}] = K^+_\Theta$ and $N^p[\bar{\Theta}] = K^p_\Theta$.

We use the notation b for the Blaschke factor

$$b(z) = \frac{\mathrm{i} - z}{\mathrm{i} + z} \; .$$

The argument $2\arctan(x)$ of b increases from $-\pi$ at $-\infty$ to $+\pi$ at $+\infty$. One can characterize the dimension of a Toeplitz kernel by multiplying the symbol by integer powers of b.

Lemma 3.1. *For $n \in \mathbb{N}$, $\dim\ N^p[U] = n + 1$ iff $\dim\ N^p[b^n U] = 1$.*

Proof. If, for instance, $\dim\ N^p[U] \geq 2$, then we can find an $F \in N^p[U]$ such that $F(\mathrm{i}) = 0$, and so $\bar{b}F \in N^p[bU]$ and $\dim\ N^p[bU] \geq 1$. In the opposite direction, if $G \in N^p[bU]$, then both G and bG are in $N^p[U]$. □

One can also consider fractional powers of b:

$$b^s(x) = \exp(2s\mathrm{i}\arctan x) \; , \qquad (s \in \mathbb{R}) \; .$$

The identity

$$\bar{b}^s(1 - b)^s = (\bar{b} - 1)^s$$

shows that $N^\infty[\bar{b}^s] \neq 0$ for $s \geq 0$. It follows that for every U and $p > 0$ there is a critical value $s_* \in \mathbb{R} \cup \{\pm\infty\}$ such that

$$N^p[\bar{b}^s U] \neq 0 \text{ if } s > s_* \; , \qquad N^p[\bar{b}^s U] = 0 \text{ if } s < s_* \; .$$

One can interpret s_* as a fractional and possibly negative "dimension" of the kernel. For example, "dim" $N[1] = -1/2$, but "dim" $N[\bar{\Theta}_N \Theta_D] = -1/4$ for the Dirichlet and Neumann inner functions (10), see Sect. 3.7 below.

3.2 Basic Criterion

The following well-known observation is extremely simple but quite useful. In fact, most of our further constructions are built upon this lemma.

Lemma 3.2. *$N^p[U] \neq 0$ iff the symbol has the following representation:*

$$U = \bar{\Phi}\frac{\bar{H}}{H} \; ,$$

where $H \in \mathcal{H}^p \cap L^1_{\mathrm{loc}}(\mathbb{R})$ is an outer function and Φ is an inner function.

Proof. If $UF = \bar{G}$, then $|F| = |G|$ on $\mathbb{R}$. Consider the inner-outer factorization: $F = F_i F_e$ and $G = G_i G_e$. We have $F_e = G_e$ and

$$U = (\bar{F}_i \bar{G}_i)\frac{\bar{F}_e}{F_e} \; .$$

The converse is obvious. □

Corollary 3.3. *If $\gamma \in L^\infty \cap C(\mathbb{R})$, then $\exists p > 0$, "dim" $N^p[\mathrm{e}^{\mathrm{i}\gamma}] > -\infty$.*

A more precise statement is

$$\|\gamma\|_\infty < \frac{\pi}{p} \quad \Rightarrow \quad N^p[\bar{b}^{2/p}\mathrm{e}^{\mathrm{i}\gamma}] \neq 0 \, ,$$

which follows from the Smirnov–Kolmogorov estimate

$$\|h\|_\infty < \frac{\pi}{2} \quad \Rightarrow \quad \mathrm{e}^{\tilde{h}} \in L^1_\Pi \, ,$$

and from the construction of outer functions.

Of course, instead of $\|\gamma\|_\infty < \infty$ we can only require that γ be the sum of a decreasing and a BMO functions, and we don't need continuity if $p \geq 1$. It is also important to realize that p can not be arbitrary in the statement of the corollary. For instance, it is easy to construct $\gamma \in C^\omega(\mathbb{R})$ such that $\|\gamma\|_\infty = \pi/2$ but $N[\bar{b}^n \mathrm{e}^{\mathrm{i}\gamma}] = 0$ for all $n > 0$.

3.3 Sufficient Conditions for $\dim N^p[u] < \infty$

The following statement is a version of Coburn's lemma, which states that either ker $T_U = 0$ or ker $T_{\bar{U}} = 0$.

Lemma 3.4. *If $1/p + 1/q > s$, then*

$$N^q[\bar{U}] \cap L^2_{\mathrm{loc}}(\mathbb{R}) \neq 0 \quad \Rightarrow \quad N^p[\bar{b}^s U] \cap L^2_{\mathrm{loc}}(\mathbb{R}) = 0 \, .$$

Proof. Suppose both kernels are non-trivial:

$$\bar{U}F_1 = \bar{G}_1 \, , \qquad \bar{b}^s U F_2 = \bar{G}_2 \, ,$$

for some $F_1, G_1 \in \mathcal{H}^q$ and $F_2, G_2 \in \mathcal{H}^p$. Then

$$(\mathrm{i} + z)^s F_1(z) F_2(z) = (\mathrm{i} - \bar{z})^s \bar{G}_1(\bar{z}) \bar{G}_2(\bar{z}) \quad \text{on } \mathbb{R} \, ,$$

so we have an entire Cartwright function with at most a polynomial growth along $\mathrm{i}\mathbb{R}$. The growth at $+\mathrm{i}\infty$ is

$$y^s y^{-1/q} y^{-1/p} \, ,$$

so the entire function is zero if $1/p + 1/q > s$. □

Corollary 3.5. *If γ is the sum of an increasing and a bounded functions, then for all $p > 0$, $\dim N^p[\mathrm{e}^{\mathrm{i}\gamma}] < \infty$.*

Corollary 3.6. *If $U = \bar{H}/H$ and H is an outer function such that*

$$\exists q > 0 \quad \exists N \, , \quad \frac{1}{H} \in L^q \left(\frac{\mathrm{d}t}{1 + |t|^N} \right) \, ,$$

then for all $p > 0$, dim $N^p[U] < \infty$.

3.4 Trivial Factors

The following lemma is obvious.

Lemma 3.7. *If $V = \bar{H}/H$ with $H^{\pm 1} \in \mathcal{H}^\infty$, then $N^p[UV] \neq 0$ iff $N^p[U] \neq 0$.*

We will call such functions V trivial factors of the symbol.

Example 3.8. If B_1 and B_2 are *finite* Blaschke products of the same degree, then $N^p[U] = 0$ iff $N^p[\bar{B}_1 B_2 U] = 0$.

Example 3.9. If we modify a smooth symbol on a compact part of $\mathbb{R}$, then this does not affect (non-)triviality of the Toeplitz kernels. Thus the injectivity property depends only on the behavior of a smooth symbol at infinity.

Example 3.10. It is shown in [9] that up to a trivial factor every unimodular function is the ratio of two inner functions.

More relevant to the subject of the paper is our next

Example 3.11 (Weyl inner functions of regular operators). Let $q \in L^1[0,1]$ and let α be a *non-Dirichlet* selfadjoint boundary condition at $a = 0$. Denote by Θ the Weyl inner function of (q, α) computed at $b = 1$, i.e. $\Theta = \Theta^b_{\alpha,a}$ in the notation of Sect. 2.4. We want to compare Θ with the "Neumann" inner function Θ_N, see (10), which corresponds to the special case $q \equiv 0$ and $\alpha = (N)$.

Claim. The ratio Θ/Θ_N is a trivial factor.

In other words, in all problems involving Toeplitz kernels we are free to replace regular potentials with the trivial potential, and any non-Dirichlet boundary condition with the Neumann condition.

Proof. We will express the ratio of the Weyl inner functions in terms of their de Branges functions. The de Branges function of Θ_N is

$$E_N(\lambda) = \cos\sqrt{\lambda} - \mathrm{i}\sqrt{\lambda}\sin\sqrt{\lambda}\ ,$$

and by (17) the de Branges function of Θ is

$$E(\lambda) = -\dot{u}(\lambda) + \mathrm{i}u(\lambda)\ , \qquad u(\lambda) := u_\lambda(1)\ , \quad \dot{u}(\lambda) := \dot{u}_\lambda(1)\ ,$$

where $u_\lambda(t)$ is the solution of the Schrödinger equation with boundary condition α and initial value $u_\lambda(0) = 1$. We have

$$\frac{\Theta}{\Theta_N} = \frac{\bar{H}}{H}\ , \qquad H = \frac{E}{E_N}\ .$$

Since both de Branges functions are outer in $\mathbb{C}_+$, all we need to check is that $|E| \asymp |E_N|$ on $\mathbb{R}$. To this end we can use the standard asymptotic formulae for solutions of a regular Schrödinger equation, see e.g. [30]:

$$|u(\lambda) - \cos\sqrt{\lambda}| = \left(\frac{1}{\sqrt{\lambda}}\right) , \qquad |\dot{u}(\lambda) + \sqrt{\lambda}\sin\sqrt{\lambda}| = O(1) , \qquad (\lambda \to \pm\infty) .$$

For instance if $q \equiv 0$ but $\alpha \neq (N)$, then

$$u(\lambda) = \frac{\cos(\sqrt{\lambda} + \psi(\lambda))}{\cos\psi(\lambda)} , \qquad \sqrt{\lambda}\tan\psi(\lambda) = \cot\frac{\alpha}{2} ,$$

and the asymptotic is obvious.

If $\lambda \to +\infty$, then

$$|E(\lambda)|^2 \ , \ |E_N(\lambda)|^2 \ \asymp [\cos\sqrt{\lambda} + O(\lambda^{-1/2})]^2 + \lambda[\sin\sqrt{\lambda} + O(\lambda^{-1/2})]^2 := I + II ,$$

and we consider three cases:

- if $|\sin\sqrt{\lambda}| \lesssim \lambda^{-1/2}$, then $I \asymp 1$ and $0 \leq II \lesssim 1$, so $I + II \asymp 1$;
- if $|\cos\sqrt{\lambda}| \lesssim \lambda^{-1/2}$, then $\sin^2\sqrt{\lambda} \approx 1$ and both $|E|^2$ and $|E_N|^2$ are $\asymp \lambda$;
- if $|\sin\sqrt{\lambda}|$ and $|\cos\sqrt{\lambda}|$ are $\gg \lambda^{-1/2}$, then $I + II \asymp \cos^2\sqrt{\lambda} + \lambda\sin^2\sqrt{\lambda}$.

The estimates for $\lambda \to -\infty$ are even easier. □

Toeplitz Kernels with Real Analytic Symbols

From now on we will be considering unimodular functions with real analytic arguments, $U = \mathrm{e}^{\mathrm{i}\gamma}$, $\gamma \in C^\omega(\mathbb{R})$. In this case, all elements of the Toeplitz kernels are also real analytic on $\mathbb{R}$.

Lemma 3.12. *If $\gamma \in C^\omega(\mathbb{R})$, then $N^+[\mathrm{e}^{\mathrm{i}\gamma}] \subset C^\omega(\mathbb{R})$.*

Proof. Let $F \in N^+[U]$ and let G_- be the analytic extension of UF to $\mathbb{C}_-$. Since $U \neq 0$ in a neighborhood of $\mathbb{R}$ and $F = U^{-1}G_-$ on $\mathbb{R}$, F can be extended to a neighborhood of $\mathbb{R}$. □

3.5 Basic Criterion in N^+

Proposition 3.13. *Let $\gamma \in C^\omega(\mathbb{R})$. Then $N^+[\mathrm{e}^{\mathrm{i}\gamma}] \neq 0$ iff γ has a representation*

$$\gamma = -\alpha + \tilde{h} ,$$

where $\alpha \in C^\omega(\mathbb{R})$ is an increasing function and $h \in L^1_\Pi$.

Proof. We first observe that $N^+[u] \neq 0$ iff

$$U = \bar{\Phi}\frac{\bar{H}}{H} \quad \text{on } \mathbb{R} , \tag{18}$$

or some outer function $H \in C^\omega(\mathbb{R})$ that does not vanish on $\mathbb{R}$, and some meromorphic inner function Φ. Indeed, suppose $N^+[U] \neq 0$. Reasoning as in Lemma 3.2, we see that

$$U = \bar{I}\frac{\bar{F}}{F} ,$$

for some meromorphic inner function I and an outer function $F \in C^\omega(\mathbb{R})$. The outer function may have zeros on the real line. Suppose the zeros are simple. Take any meromorphic inner function J such that $\{J = 1\} = \{F = 0\}$. Then the outer function

$$H = \frac{F}{1 - J} \tag{19}$$

is zero-free on $\mathbb{R}$ and

$$U = \bar{I}\frac{1 - \bar{J}}{1 - J}\frac{\bar{H}}{H} = -\bar{I}\bar{J}\frac{\bar{H}}{H} := \bar{\Phi}\frac{\bar{H}}{H} .$$

If F has multiple zeros, then we simply repeat this reasoning taking care of the convergence.

Next we restate (18) in terms of the arguments of the involved functions. Since H is an outer function, it has the following representation:

$$H = \mathrm{e}^{-(h+\mathrm{i}\tilde{h})/2} , \qquad h \in L^1_\Pi ,$$

and since H is zero free we have $\tilde{h} \in C^\omega(\mathbb{R})$. It follows that $\gamma = -\phi + \tilde{h}$, where ϕ is a continuous argument of Φ. Since ϕ is strictly increasing, this gives the "only if" part of the theorem. To prove the "if" part, we observe that given an increasing function α, we can find an inner function with argument ϕ such that

$$\beta := \alpha - \phi \in L^\infty(\mathbb{R}) ,$$

so

$$\gamma = -\alpha + \tilde{h} = -\phi - \beta + \tilde{h} = -\phi + \tilde{h}_1 , \qquad h_1 := h + \tilde{\beta} .$$

□

3.6 Basic Criterion in $\mathcal{H}^p$

Proposition 3.14. *Let $U = \mathrm{e}^{\mathrm{i}\gamma}$ with $\gamma \in C^\omega(\mathbb{R})$. Then $N^p[U] \neq 0$ iff*

$$U = \bar{\Phi}\frac{\bar{H}}{H} ,$$

where H is an outer function in $\mathcal{H}^p \cap C^\omega(\mathbb{R})$, $H \neq 0$ on $\mathbb{R}$ and Φ is a meromorphic inner function. Alternatively, $N^p[U] \neq 0$ iff

$$\gamma = -\phi + \tilde{h} , \qquad h \in L^1_\Pi , \qquad \mathrm{e}^{-h} \in L^{p/2}(\mathbb{R}) , \tag{20}$$

where ϕ is the argument of some meromorphic inner function.

To prove the statement we just repeat the previous proof using the following lemma, in which we construct the Herglotz measure of a meromorphic inner function J so that the function H in (19) in the previous proof belongs to $\mathcal{H}^p$.

Lemma 3.15. *If $0 < p \le \infty$ and $F \in \mathcal{H}^p \cap C^\omega(\mathbb{R})$, then there is a finite positive measure ν supported exactly on $\{F = 0\} \cap \mathbb{R}$ such that*

$$F \cdot \mathcal{S}\nu \in \mathcal{H}^p \cap C^\omega(\mathbb{R}) \,, \qquad \mathcal{S}\nu(z) := \int \frac{\mathrm{d}\nu(t)}{t-z} \,.$$

Proof. Let $\{b_k\}$ be all real zeros of F; we assume for simplicity that the zeros are simple. Choose small positive numbers ϵ_k,

$$\sum \epsilon_k < 1 \,, \tag{21}$$

such that the ϵ_k–neighborhoods of b_k are disjoint. We have

$$|F(z)| \le C_k |z - b_k| \,,$$

if z is in the ϵ_k-neighborhood of b_k. Take

$$\nu = \sum \nu_k \delta_{b_k} \,, \qquad \nu_k = C_k^{-1} 2^{-k} \epsilon_k \,,$$

and observe that

$$|\mathcal{S}\nu(z)| \le \sum_k \frac{\nu_k}{|z - b_k|} \,.$$

If z is outside of all neighborhoods, then

$$|F\mathcal{S}\nu|(z) \le |F(z)| \sum 2^{-k} = |F(z)| \,.$$

If z is in the k:th neighborhood, then

$$|F\mathcal{S}\nu|(z) \le |F(z)| + \frac{|F(z)|\nu_k}{|z - b_k|} \le |F(z)| + C_k\nu_k \le |F(z)| + 1 \,.$$

We have $F\mathcal{S}\nu \in \mathcal{H}^p$ by (21). □

3.7 Kolmogorov–Type Criterion

The basic criterion is particularly useful in the case when we can represent γ as the argument of some explicitly given outer function, e.g., when U is the ratio of two inner functions with known de Branges functions.

Proposition 3.16. *Let $U = \bar{H}/H$, and H is an outer function real analytic and zero free on $\mathbb{R}$. Suppose* $\dim N^p[U] < \infty$. *Then*

$$N^p[U] \ne 0 \quad \Leftrightarrow \quad H \in \mathcal{H}^p \,.$$

Proof. If $N^p[U] \ne 0$, then $\dim N^p[b^s U] = 1$ for some $s \ge 0$. We have

$$b^s U = \bar{H}_s / H_s \,, \qquad H_s = (1-b)^{-s} H \,.$$

By Proposition 3.14 we have a representation

$$\bar{H}_s/H_s = \bar{F}/F ,$$

for some outer function $F \in \mathcal{H}^p \cap C^\omega(\mathbb{R})$, $F \neq 0$ on $\mathbb{R}$. Since the function H_s is also outer and zero-free, it follows that $H = \mathrm{const}(1-b)^s F$ and so $H \in \mathcal{H}^p$. The converse is trivial. □

Remark 3.17. If $p = 2$ and $1/H \in H^2$, then the proof shows that the conclusion is true even without the assumption $H \in C^\omega(\mathbb{R})$. The corresponding statement in the unit disc is equivalent to Kolmogorov's minimality criterion in the theory of stationary Gaussian processes: $\{z^n\}$ is minimal in $L^2(w)$ iff $w^{-1} \in L^1$.

Remark 3.18. The condition dim $N^p[u] < \infty$ is essential and related to the concept of "rigid functions", see [37]. We already mentioned two sufficient conditions for dim $N^p[u] < \infty$ in Sect. 3.3.

Example 3.19. This simple example is meant to illustrate the above criterion. Let Θ_D and Θ_N be the Weyl inner functions (10) for potential $q = 0$ on $[0,1]$ with Dirichlet and Neumann boundary conditions at 0. We claim that the "fractional dimension" of the kernel $N[\bar{\Theta}_N \Theta_D]$ is $-1/4$, see Sect. 3.1.

Proof. We represent the ratio Θ_D/Θ_N in terms of de Branges functions:

$$\frac{\Theta_D}{\Theta_N} = \frac{\bar{H}}{H} , \qquad H = \frac{E_D}{E_N} ,$$

where

$$E_N(\lambda) = \cos\sqrt{\lambda} - \mathrm{i}\sqrt{\lambda}\sin\sqrt{\lambda} , \qquad E_D(\lambda) = \frac{\sin\sqrt{\lambda}}{\sqrt{\lambda}} + \mathrm{i}\cos\sqrt{\lambda} ,$$

so

$$U := \frac{\bar{H}}{H} , \qquad H = \frac{1}{\sqrt{\lambda}} \frac{\sin\sqrt{\lambda} + \mathrm{i}\sqrt{\lambda}\cos\sqrt{\lambda}}{\cos\sqrt{\lambda} - \mathrm{i}\sqrt{\lambda}\sin\sqrt{\lambda}} .$$

Clearly, $\dim N[U] < \infty$, and by Kolmogorov's criterion we have $N[\bar{b}^s U] \neq 0$ iff $F := (1-b)^s H \in L^2(\mathbb{R})$. If $x > 0$, then

$$|H(x)|^2 = \frac{1}{x} \frac{\sin^2\sqrt{x} + x\cos^2\sqrt{x}}{\cos^2\sqrt{x} + x\sin^2\sqrt{x}} .$$

Let us estimate $|F|^2$ on an interval I_n about $\pi^2 n^2$ where $|\sin\sqrt{x}| \ll 1$. If we write $x = \pi^2 n^2 + s$, so

$$|\sqrt{x} - \pi n| \asymp \frac{|s|}{n} , \qquad \sin^2\sqrt{x} \asymp \frac{s^2}{n^2} , \qquad x\sin^2\sqrt{x} \asymp s^2 ,$$

then

$$|H(x)|^2 \asymp \frac{1}{x}\,\frac{x}{1+x\sin^2\sqrt{x}} \asymp \frac{1}{1+s^2}\,,$$

$$|F(x)|^2 \asymp n^{-4s}\frac{1}{1+s^2}\,, \qquad \int_{I_n} |F|^2 \asymp n^{-4s}\,.$$

Thus $F \in L^2(\mathbb{R}_+)$ iff $4s > 1$. Finally we note that

$$|H(x)| \sim \frac{1}{\sqrt{|x|}}\,, \qquad x \to -\infty\,,$$

and so $F \in L^2(\mathbb{R}_-)$ iff $s > 0$. □

Similarly one can show that "dim" $N[\bar{\Theta}_D \Theta_N] = -5/4$. One can also compute the dimensions of kernels in other Hardy spaces. In particular, "dim" $N^\infty[\bar{\Theta}_N \Theta_D] = 0$ and "dim" $N^\infty[\bar{\Theta}_D \Theta_N] = -1$; moreover, $N^\infty[\bar{\Theta}_N \Theta_D] \neq 0$ and $N^\infty[\bar{b}\bar{\Theta}_D \Theta_N] \neq 0$.

3.8 Twin Inner Functions

We say that two meromorphic inner functions are *twins* if they have the same point spectrum (possibly including infinity). Twin functions appear in several applications (see, e.g., Sect. 4.5 below), and the main result is that the Toeplitz operator corresponding to their ratio is injective. This fact is quite different from Levinson's type conditions discussed later in this section.

Theorem 3.20. *Let Θ and J be twin meromorphic inner functions. Then $N[\bar{\Theta}J] = 0$.*

Proof. We have

$$\bar{\Theta}J = \frac{\bar{H}}{H}\,, \qquad H = \frac{1-\Theta}{1-J}\,.$$

Since $H^{\pm 1} \in C^\omega(\mathbb{R})$, we can apply Kolmogorov's criterion. (The kernel is finite dimensional because the argument of $\bar{\Theta}J$ is bounded.) We claim that $H \notin \mathcal{H}^2$. Indeed, if Θ has no point mass at infinity, then

$$|H| \geq \frac{1}{2}|1-\Theta| \notin L^2\,.$$

If both functions have a point mass at infinity, then by l'Hôpital's rule the angular limit

$$\lim_{\infty} \frac{1-\Theta}{1-J} = \frac{\Theta'(\infty)}{J'(\infty)}$$

exists and is non-zero (see Sect. 2.2), so H can not be in $\mathcal{H}^2$. □

Remark 3.21. The proof shows that $N[\bar{\Theta}J] = 0$ if we have $\{\Theta = 1\} = \{J = 1\}$ and $\infty \notin \sigma(\Theta)$. Moreover, it can be shown that

$$\sigma(\Theta) \subset \sigma(J) \quad \Rightarrow \quad N[\bar{\Theta}J] = 0\,.$$

Remark 3.22. Similar technique applies to symbols of the form $u = \bar{\Theta} J \bar{H}/H$ where Θ and J are twin inner functions, and H is an outer function real-analytic and zero free on $\mathbb{R}$. If dim $N^p[\bar{H}/H] < \infty$, then

$$N^p[\bar{b}^s \bar{\Theta} J \bar{H}/H] \neq 0 \quad \Leftrightarrow \quad (1-b)^s \frac{1-\Theta}{1-J} H \in H^p \ .$$

General Form of Levinson's Completeness Theorem

As we mentioned in Sect. 3.1, if $\exists\ \gamma(\pm\infty)$, then

$$\delta = \gamma(+\infty) - \gamma(-\infty) > -\frac{2\pi}{p} \quad \Rightarrow \quad N^p[\mathrm{e}^{\mathrm{i}\gamma}] = 0 \ , \qquad (0 < p < \infty) \ .$$

We extend this fact to general symbols by considering the "mean" behavior at $+\infty$ of the function

$$\delta(x) = \gamma(x) - \gamma(-x) \ .$$

Our result has the same form as Kolmogorov's type condition in Sect. 4.7, but this time we don't assume a priory that the kernel is finite dimensional. The new idea is to apply the Poisson A–integral transform to the equation (20) in the basic criterion. (See Sect. 4.4 for another application of this idea.)

3.9 Titchmarsh and Uly'anov Theorems

Let $h \in L^1_{\mathrm{loc}}(\mathbb{R})$ be a real valued function. For each $A > 0$ we denote

$$h^A = \begin{cases} h(x) & |h(x)| \leq A \ , \\ 0 & |h(x)| \geq A \ . \end{cases}$$

The Schwarz A–integral of h is defined by the formula

$$\mathcal{S}_{(A)} h(z) = \lim_{A \to \infty} \ \mathcal{S} f^A(z) \ , \qquad z \in \mathbb{C}_+ \ ,$$

provided that the limit exists for all z. Similarly, one defined the Poisson and the conjugate Poisson A–integrals $\mathcal{P}_{(A)} h$ and $\mathcal{Q}_{(A)} h$ respectively so that

$$\mathcal{S}_{(A)} h = \mathcal{P}_{(A)} h + \mathrm{i} \mathcal{Q}_{(A)} h \ .$$

Recall that if $h, \tilde{h} \in L^1_{\Pi}$, then $\mathcal{S}\tilde{h} = -\mathrm{i}\mathcal{S}h + \mathrm{i}\mathcal{S}h(\mathrm{i})$.

Theorem 3.23. *If $h \in L^1_{\Pi}$, then the Schwarz A–integral of $\tilde{h}$ exists, and we have*

$$\mathcal{S}_{(A)} \tilde{h}(z) = -\mathrm{i}\mathcal{S}h(z) + \mathrm{i}\mathcal{S}h(\mathrm{i}) \ , \qquad z \in \mathbb{C}_+ \ . \tag{22}$$

The real part of the equation (22), or rather its special case

$$\mathcal{P}_{(A)}\tilde{h}(\mathrm{i}) = 0 \, , \tag{23}$$

is due to Titchmarsh, see [42], and the imaginary part of (22),

$$Q_{(A)}\tilde{h} = -Ph + Ph(\mathrm{i}) \, , \tag{24}$$

is the Uly'anov's theorem, see [2] for a shorter proof. Note that we use a slightly different definition of the A–transforms but the definitions are in fact equivalent because $\tilde{h} \in L^{o(1,\infty)}_{\Pi}$.

3.10 A Sufficient Condition for $N^p[U] = 0$

For an odd function $\delta : \mathbb{R} \to \mathbb{R}$ we define

$$L\delta(y) = \frac{2}{\pi}\int_0^\infty \left[\frac{1}{1+t^2} - \frac{1}{y^2+t^2}\right] t\delta(t)\,\mathrm{d}t \, , \qquad y > 0 \, .$$

The integral makes sense (it might be $\pm\infty$) if we assume that

$$\text{either} \int^\infty \delta^+(t)\, t^{-3}\mathrm{d}t < \infty \qquad \text{or} \int^\infty \delta^-(t)\, t^{-3}\mathrm{d}t < \infty \, , \tag{25}$$

where, as usual, $\delta^\pm := \max\{\pm\delta, 0\}$. Note that if $\delta \in L^1_\Pi$, then $L\delta(y) = \tilde{\delta}(\mathrm{i}y)$.

Theorem 3.24. *Let $\gamma \in C^\omega(\mathbb{R})$ and let $\delta(x) = \gamma(x) - \gamma(-x)$ satisfy* (25). *Then*

$$N^p[\mathrm{e}^{\mathrm{i}\gamma}] \neq 0 \quad \Rightarrow \quad \exists F \in \mathcal{H}^{p/4}(\mathbb{C}_+), \quad \mathrm{e}^{L\delta(y)} \leq |F(iy)|, \quad (y > 1) \, .$$

Proof. By (20) we have

$$\gamma = -\phi + \tilde{h}_1 \, , \qquad h_1 \in L^1_\Pi, \quad \mathrm{e}^{-h_1} \in L^{p/2} \, .$$

Then

$$-\gamma(-x) = \phi(-x) + \tilde{h}_2(x) \, , \qquad h_2 \in L^1_\Pi, \quad \mathrm{e}^{-h_2} \in L^{p/2} \, .$$

It follows that

$$\delta = -\psi + \tilde{h} \, , \qquad h \in L^1_\Pi, \quad \mathrm{e}^{-h} \in L^{p/4} \, ,$$

where ψ is an *odd* increasing function. We apply the Uly'anov theorem to

$$\tilde{h} = \delta_1 := \psi + \delta \, .$$

By (24) we have

$$\mathcal{Q}_A\delta_1 = \mathcal{Q}_A\tilde{h} = -\mathcal{P}h + \text{const} \, ,$$

so

$$e^{\mathcal{Q}_A\delta_1} = \text{const}\,|F|\,, \qquad F := e^{-\mathcal{S}h} \in \mathcal{H}^{p/4}$$

and it remains to show that

$$L\delta(y) \le \mathcal{Q}_A\delta_1(\mathrm{i}y)\,.$$

Since $t\delta_1(t) \ge t\delta(t)$ for all $t \in \mathbb{R}$, and since the kernel of L is positive for $y > 1$, we have

$$\begin{aligned}
\pi\mathcal{Q}_A\delta_1(\mathrm{i}y) &= \lim_{A\to\infty}\int_{\{|\delta_1|<A\}}\left[\frac{1}{1+t^2} - \frac{1}{y^2+t^2}\right] t\delta_1(t)\;\mathrm{d}t \\
&\ge \lim_{A\to\infty}\int_{\{|\delta_1|<A\}}\left[\frac{1}{1+t^2} - \frac{1}{y^2+t^2}\right] t\delta(t)\;\mathrm{d}t \\
&= \int_{\mathbb{R}}\left[\frac{1}{1+t^2} - \frac{1}{y^2+t^2}\right] t\delta(t)\;\mathrm{d}t = \pi L\delta(y)\,.
\end{aligned}$$

□

Remark 3.25. The proof works for any γ such that

$$\gamma = -\phi + \tilde{h}\,, \qquad h \in L^1_{\Pi}, \quad e^{-h} \in L^{p/2}\,.$$

We don't need to assume $\gamma \in C^\omega$ as long as we have such a representation.

3.11 Levinson–Type Conditions

We can use standard growth estimates of Hardy space functions to derive more familiar looking conditions.

Condition (a).

$$N^p[e^{\mathrm{i}\gamma}] \ne 0 \quad\Rightarrow\quad e^{L\delta(y)} = o\left(y^{-4/p}\right)\,, \qquad y \to +\infty\,,$$

In other words,

$$\limsup_{y\to\infty}\left[L\delta(y) + \frac{4}{p}\log y\right] > -\infty \quad\Rightarrow\quad N^p[u] = 0\,. \tag{26}$$

Example 3.26. A simple computation shows

$$[L\ \mathrm{sign}](y) = \frac{2}{\pi}\log y\,.$$

It follows that $N[e^{\mathrm{i}\gamma}] = 0$ if $\gamma(x) \ge \gamma(-x) - \pi$ for $x \ge x_0$. Indeed, we have $\delta \ge -\pi$ for large x, and therefore

$$L\delta(y) \ge -\pi[L\ \mathrm{sign}](y) + O(1) = -2\log y + O(1)\,.$$

Condition (b).

$$N^p[\mathrm{e}^{\mathrm{i}\gamma}] \neq 0 \quad \Rightarrow \quad \int^{\infty} \mathrm{e}^{pL\delta(y)/4}\mathrm{d}y < \infty \; .$$

For example,

$$L\delta(y) \geq -\frac{4}{p}\log y - \log\log y \quad \Rightarrow \quad N^p[\mathrm{e}^{\mathrm{i}\gamma}] = 0 \; .$$

A more general statement is

$$N^p[\mathrm{e}^{\mathrm{i}\gamma}] \neq 0 \quad \Rightarrow \quad \int_0^{\infty} \mathrm{e}^{pL\delta(y)/4}\mathrm{d}\nu(y) < \infty \; ,$$

for any Carleson measure ν in $\mathbb{C}_+$.

Condition (c). For each $y > 1$, the quantity

$$\frac{L\delta(y)}{[L\ \mathrm{sign}](y)} = \frac{\pi}{2}\,\frac{L\delta(y)}{\log y}$$

is some sort of "averaging" of δ near $+\infty$. The meaning of (26) is that the "mean" value of δ in infinity has to be "less" than $-2\pi/p$ for the Toeplitz kernel $N^p[\mathrm{e}^{\mathrm{i}\gamma}]$ to be non-trivial. Here is a different way to express the same idea.

Corollary 3.27. *Suppose $\delta(x)$ satisfies the integrability conditions* (25)*. Then $N^p[\mathrm{e}^{\mathrm{i}\gamma}] = 0$ if*

$$\int_0^x \frac{\delta(t)}{t}\mathrm{d}t \geq -\frac{2\pi}{p}\log x + O(1) \; , \qquad x \to +\infty \; .$$

Proof. Integration by parts shows: if

$$\int_0^x \frac{a(t)}{t}\mathrm{d}t \leq \log x + O(1) \; , \qquad x \to \infty \; ,$$

then

$$\int_0^{\infty} \frac{y^2}{y^2+t^2}\,\frac{a(t)\mathrm{d}t}{t} \leq \log y + O(1) \; , \qquad y \to \infty \; .$$

(If the latter integral is not converging, then we understand it as $\limsup \int_0^x .$) $\square$

4 Some Applications

Completeness and Minimality Problem

4.1 Restatement in Terms of Uniqueness Sets and Toeplitz Kernels

We will study the following situation. Consider the Schrödinger equation (2) on an interval (a, b) with potential q and some fixed selfadjoint boundary condition β at b. We assume that the endpoint a is regular. For each $\lambda \in \mathbb{C}$ we choose a non-trivial solution u_λ satisfying the boundary condition; this solution is unique up to a constant. If $\Lambda \subset \mathbb{C}$, we say that the family $\{u_\lambda\}_{\lambda\in\Lambda}$ is *complete* if

$$\operatorname{span}\{u_\lambda : \lambda \in \Lambda\} = L^2(a,b) ,$$

and is *minimal* if

$$\forall \lambda_0 \in \Lambda, \quad u_{\lambda_0} \notin \operatorname{span}\{u_\lambda : \lambda \in \Lambda \setminus \lambda_0\} .$$

We will use the notation of Sects. 2.4 and 2.6: $\Theta = \Theta^a_{b,\beta}$ is the Weyl inner function, and E is a de Branges function of Θ. For $\lambda \in \mathbb{C}_+ \cup \mathbb{R}$ we have reproducing kernels k_λ and dual reproducing kernels k^*_λ of K_Θ, see (13). For $\lambda \in \mathbb{C}$, let K^E_λ denote the reproducing kernel in $B(E)$. Finally, we represent

$$\Lambda = \Lambda_+ \cup \Lambda_- , \qquad \Lambda_+ := \Lambda \cap (\mathbb{C}_+ \cup \mathbb{R}), \quad \Lambda_- := \Lambda \cap \mathbb{C}_- .$$

Lemma 4.1. *The following assertions are equivalent:*

(i) the family $\{u_\lambda\}_{\lambda\in\Lambda}$ is complete (minimal) in $L^2(a,b)$;
(ii) the family $\{K^E_{\bar\lambda}\}_{\lambda\in\Lambda}$ is complete (minimal) in $B(E)$;
(iii) the family $\{k_{\bar\lambda}\}_{\lambda\in\Lambda_-} \cup \{k^*_\lambda\}_{\lambda\in\Lambda_+}$ is complete (minimal) in K_Θ.

Proof. This follows from Theorem 2.3 and Corollary 2.9. □

We say that $\Lambda \subset \mathbb{C}$ is a *uniqueness set* of $B(E)$ if there is no non-trivial function $F \in B(E)$ such that $F = 0$ on Λ. The equivalence $(i) \Leftrightarrow (ii)$ in the above lemma means that $\{u_\lambda\}_{\lambda\in\Lambda}$ is complete if and only if Λ is a uniqueness set of $B(E)$, and that $\{u_\lambda\}_{\lambda\in\Lambda}$ is minimal if and only if $\Lambda \setminus \lambda_0$ is not a uniqueness set for any $\lambda_0 \in \Lambda$.

We define uniqueness sets Λ of K_Θ in a similar way; in this case $\Lambda \subset \mathbb{C}_+ \cup \mathbb{R}$. The definition obviously extends to *divisors*, i.e. sets of points with assigned multiplicities.

Lemma 4.2. *Let $\Lambda \subset \mathbb{C}_+ \cup \mathbb{R}$ and let $M \subset \mathbb{C}_+$. Then the family*

$$\{k_\lambda\}_{\lambda\in\Lambda} \cup \{k^*_\mu\}_{\mu\in M}$$

is complete in K_Θ if and only if $\Lambda \cup M$ is a uniqueness divisor.

Proof. Suppose the family is not complete, so there is a non-trivial $F \in K_\Theta$ orthogonal to all k_λ and k^*_μ. Let $H \in K_\Theta$ be defined by the relation

$$\bar\Theta F = \bar H \quad \text{on } \mathbb{R} .$$

Then we have $F = 0$ on Λ and $H = 0$ on M. (Recall that $\bar\Theta k_\mu = k^*_\mu$.) From the latter fact we have a representation

$$H = B_M G , \qquad G \in \mathcal{H}^2 ,$$

where B_M is the Blaschke product, and therefore

$$\bar{\Theta}(B_M F) = \bar{G}\ .$$

The function $B_M F$ is in K_Θ and is zero on $\Lambda \cup M$. The opposite direction is similar. $\square$

The equivalence $(i) \Leftrightarrow (iii)$ in the first lemma now means that $\{u_\lambda\}_{\lambda\in\Lambda}$ is complete in $L^2(a,b)$ if and only if $\Lambda_+ \cup \overline{\Lambda_-}$ is a uniqueness divisor of $B(E)$. The characterization of minimality is similar.

It is very easy to characterize uniqueness sets (or divisors) Λ of K_Θ in the terms of Toeplitz kernels in the case $\Lambda \subset \mathbb{C}_+$. (The case $\Lambda \subset \mathbb{R}$ is discussed in the next subsection.) A necessary and sufficient condition for uniqueness is the following:

$$N[\bar{\Theta} B_\Lambda] = 0\ .$$

Indeed, $f \in K_\Theta$ is zero on Λ if and only if $g = \bar{B}_\Lambda f \in N[\bar{\Theta} B_\Lambda]$.

Let us summarize the above discussion.

Theorem 4.3. *Let $\Lambda = \Lambda_+ \cup \Lambda_-$, $\Lambda_\pm \subset \mathbb{C}_\pm$, and let B denote the Blaschke product corresponding to the divisor $\Lambda_+ \cup \overline{\Lambda_-}$. The family $\{u_\lambda\}_{\lambda\in\Lambda}$ is complete in $L^2(a,b)$ iff $N[\bar{\Theta}B] = 0$ and is minimal iff $N[\bar{b}\bar{\Theta}B] \neq 0$. The family is complete and minimal if and only if*

$$\dim\ [\bar{b}\bar{\Theta}B] = 1\ .$$

The "dimension" of the kernel, which may be negative, see Sect. 3.1, can be interpreted as the excess/deficiency of the family.

4.2 Uniqueness Sets of K^p_Θ

We will consider the case of an arbitrary $p > 0$. As we explained, if $\Lambda \subset \mathbb{C}_+$, then

$$\Lambda \text{ is a uniqueness set of } K^p_\Theta \quad \Leftrightarrow \quad N^p[\bar{\Theta}B] = 0\ . \tag{27}$$

Now we concentrate on the case $\Lambda \subset \mathbb{R}$.

Proposition 4.4. *Let Θ be a meromorphic inner function and $\Lambda \subset \mathbb{R}$. Then Λ is a uniqueness set of K^p_Θ if and only if $N^p[\bar{\Theta}J] = 0$ for every meromorphic inner function J such that $\{J = 1\} = \Lambda$.*

Proof. Suppose we have a non-trivial function $F \in K^p_\Theta$ which is zero on Λ. By Lemma 3.15, we can find an inner function J with $\{J = 1\} = \Lambda$ such that

$$G = \frac{F}{1 - J} \in \mathcal{H}^p\ .$$

Then $G \in K^p_\Theta$, and we have

$$\bar{\Theta}JG = \bar{\Theta}(G - F) = \bar{\Theta}F\frac{J}{1-J} = -\frac{\bar{\Theta}F}{1-\bar{J}} \in \bar{\mathcal{H}}^p ,$$

so the Toeplitz kernel is non-trivial.

Conversely, if G is a non-trivial element of $N^p[\bar{\Theta}J]$, then $F = (1-J)G \in K^p_\Theta$, and so Λ is not a uniqueness set. Indeed, since $G \in N^p[\bar{\Theta}J]$, we have $JG \in K^p_\Theta$, and therefore $G \in K^p_\Theta$ and $G - JG \in K^p_\Theta$. □

Compared to the case $\Lambda \subset \mathbb{C}_+$, the condition in the last lemma seems to be less useful since it involves an infinite set of inner functions J. Nevertheless, we can overcome this difficulty and restate the criterion in both cases $\Lambda \subset \mathbb{C}_+$ and $\Lambda \subset \mathbb{R}$ in a unified way.

If $\Lambda \subset \mathbb{C}_+$, then combining (27) and (20) we see that Λ is not a uniqueness set of K^p_Θ iff the function

$$\gamma = \arg B_\Lambda - \arg \Theta \tag{28}$$

has a representation

$$\gamma = -\phi + \tilde{h} , \qquad h \in L^1_\Pi, \quad \mathrm{e}^{-h} \in L^{p/2} ,$$

where ϕ is the argument of a meromorphic inner function.

In the case $\Lambda \subset \mathbb{R}$, we will use the *counting function* n_Λ of Λ instead of the argument function of B_Λ in (28). By definition,

$$n_\Lambda = \sum n_\lambda , \qquad n_\lambda = \begin{cases} \chi(\lambda, +\infty) & \lambda > 0 , \\ -\chi(-\infty, \lambda) & \lambda < 0 . \end{cases} \tag{29}$$

Theorem 4.5. *Let Θ be a meromorphic inner function and $\Lambda \subset \mathbb{R}$. Then Λ is not a uniqueness set of K^p_Θ if and only if the function*

$$\gamma = 2\pi n_\Lambda - \arg \Theta$$

has a representation

$$\gamma = -\phi + \tilde{h} , \qquad h \in L^1_\Pi, \quad \mathrm{e}^{-h} \in L^{p/2} , \tag{30}$$

where ϕ is the argument of a meromorphic inner function.

Proof. If Λ is not a uniqueness set, then by the last proposition there is a meromorphic inner function J such that $\{J = 1\} = \Lambda$ and such that the kernel $N^p[\bar{\Theta}J]$ contains an *outer* function G which has no zeros on $\mathbb{R}$. We have

$$\bar{\Theta}J = -\bar{\Phi}\frac{\bar{G}}{G}$$

for some inner function Φ, and if we denote $F = (1-J)G$, then

$$\Theta = \Phi\frac{F}{\bar{F}} = \Phi \exp(2\mathrm{i}(\log|F|)^\sim) = \Phi \exp(\mathrm{i}[2(\log|F|)^\sim + 2\pi n_\Lambda]) .$$

The key observation is that the function in the square brackets is continuous – this follows from the fact that F is an outer function with zero set Λ, and from the identity $(\log|x|)^{\sim} = \pi\chi_{\mathbb{R}_-}$. We conclude that

$$\gamma = -\phi + \tilde{h} \, , \qquad h := -2\log|F| \, ,$$

which proves one half of the statement. Reversing the argument we get the second half. □

Example 4.6. Λ is a uniqueness set of $K^p[S^a]$ if $\gamma(t) = 2\pi n_\Lambda(t) - at$ has a representation (30). As in Sect. 3.10 consider the function

$$\delta(t) = \gamma(t) - \gamma(-t) = 2\pi N(t) - 2at \, , \qquad N(t) = \#[\Lambda \cap (-t,t)] \, .$$

Applying Corollary 3.27 (and also Remark 3.25) we get a sufficient condition

$$\int_1^x \frac{N(t)}{t} \mathrm{d}t \geq \frac{a}{\pi} x - \frac{1}{p} \log x + O(1) \, , \qquad (x \to +\infty) \, .$$

In fact, Theorem 3.24 implies the latter condition in the lim sup sense, as well as some other sufficient conditions. Similar results can be stated for various families of special functions.

Zero Sets of Entire Functions

4.3 Exact Zero Sets of $B^+(E)$–Functions

We will be considering general Cartwright–de Branges spaces, see Sect. 2.7. A set $\Lambda \subset \mathbb{C}$ is said to be an *exact zero set* of $B^+(E)$ if there exists an entire function $F \in B^+(E)$ such that $F = 0$ exactly on Λ. We'll restrict the discussion to the case $\Lambda \subset \mathbb{R}$.

Recall that $B^+(E) = EK^+(\Theta)$ where $\Theta = \Theta_E = E^\#/E$, so $\Lambda \subset \mathbb{R}$ is also an exact zero set of $K^+(\Theta)$. The following description is essentially our basic criterion in Proposition 3.13. In the next subsection we will see that in the special case $E = S^{-a}$, this description contains main results of the theory of Cartwright's functions. As usual, S denotes the singular inner function $\mathrm{e}^{\mathrm{i}z}$.

Theorem 4.7. *$\Lambda \subset \mathbb{R}$ is an exact zero set of $B^+(E)$ if and only if*

$$2\pi n_\Lambda - \arg\ \Theta_E = -bx + \tilde{h} \, , \qquad h \in L^1_\Pi, \quad b \geq 0 \, .$$

Proof. We need to show that a function $F \in B^+(E)$ with zero set Λ exists if and only

$$\Theta = JS^b \frac{H}{\bar{H}} \, , \tag{31}$$

for some inner function J with $\{J = 1\} = \Lambda$, some $b \geq 0$, and some outer function $H \in C^\omega(\mathbb{R})$ which has no zeros on $\mathbb{R}$.

$\Leftarrow$: The function

$$F(z) = \begin{cases} (1-J(z))\ H(z)E(z)S^b(z) & z \in \mathbb{C}_+ , \\ (J^\#(z)-1)\ H^\#(z)E^\#(z) & z \in \mathbb{C}_- , \end{cases}$$

is in $B^+(E)$ and vanishes exactly on Λ.

$\Rightarrow$: Suppose $F \in B^+(E)$ vanishes exactly on Λ. Since $B^+(E) = EK^+_\Theta$, there is $G \in K^+_\Theta$ such that $F = EG$ in $\mathbb{C}_+$. Clearly, we can assume that G is an outer function. Define $G_- \in N^+(\mathbb{C}_+)$ by the equation

$$\bar{\Theta}G = \bar{G}_- \quad \text{on } \mathbb{R} .$$

Since

$$F(z) = E^\#(z)\overline{G_-(\bar{z})} , \qquad z \in \mathbb{C}_- ,$$

G_- has no zeros in C_+, and therefore its inner-outer factorization has the form

$$G_- = S^b G , \qquad b \geq 0 . \tag{32}$$

We now take any meromorphic inner function J with $\{J = 1\} = \Lambda$ and define

$$H = \frac{G}{1-J} .$$

This is an outer function with the stated properties. We have

$$G = H(1-J) , \qquad G_- = H(1-J)S^b ,$$

and from (32) we get the representation (31). □

Example 4.8. $\Lambda \subset \mathbb{R}$ is an exact zero set of a Cartwright function if and only if

$$n_\Lambda(x) = cx + \tilde{h} , \qquad c \geq 0 , \quad h \in L^1_\Pi . \tag{33}$$

4.4 Zeros of Cartwright's Functions

We need the following elementary lemma.

Lemma 4.9. *Suppose* $g \in L^{o(1,\infty)}_\Pi$ *and* $g' \geq -\text{const}$. *Then*

$$g(x) = o(x) , \qquad x \to \pm\infty .$$

Proof. If $g(x_*) \geq cx_*$, $x_* \gg 1$, then for $x > x_*$ we have (assuming $g' \geq -1$)

$$g(x) \geq g(x_*) - (x - x_*) \geq (1+c)x_* - x ,$$

and so $g(x) \gtrsim x_*$ on an interval $[x_*, (1+\delta)x_*]$. The Poisson measure of this interval is $\asymp 1/x_*$, which contradicts the weak L^1-condition. □

Corollary 4.10. *Let $\Lambda \subset \mathbb{R}$ be the exact zero set of some Cartwright function. Then*

$$\exists c \geq 0 \ , \qquad \lim_{x \to -\infty} \frac{n_\Lambda(x)}{x} = \lim_{x \to +\infty} \frac{n_\Lambda(x)}{x} = c.$$

Proof. From (33) we conclude that $g(x) = n_\Lambda(x) - cx$ satisfied the conditions of the lemma. □

Corollary 4.11. *If $\Lambda \subset \mathbb{R}$ is the exact zero set of a Cartwright function, then there exists a limit*

$$\text{v.p.} \sum_{\lambda \in \Lambda} \frac{1}{\lambda} \ .$$

Proof. For every $B > 0$ we define the function

$$\eta_B(t) = \begin{cases} B & t > B \ , \\ t & t \in [-B, B] \ , \\ -B & t < -B \ . \end{cases}$$

Using the notation (29), we have

$$\sum_{|\lambda| \leq B} n_\lambda = n_\Lambda \circ \eta_B \ .$$

We also introduce an elementary function

$$g(\lambda) = \int n_\lambda d\Pi = \frac{\pi}{2}\text{sign}(\lambda) - \arctan \lambda = \frac{1}{\lambda} + O\left(\frac{1}{\lambda^2}\right) \ , \qquad \lambda \to \pm\infty \ .$$

By the previous corollary we have

$$\exists \quad \text{v.p.} \sum \frac{1}{\lambda} \quad \Leftrightarrow \quad \exists \quad \text{v.p.} \sum g(\lambda) \ .$$

By (33), $n_\Lambda = cx + f$, where we write f for $\tilde{h}$, and therefore

$$\sum_{|\lambda| \leq B} g(\lambda) = \int n_\Lambda \circ \eta_B \ \mathrm{d}\Pi = \int f \circ \eta_B \ \mathrm{d}\Pi + \text{const} \ .$$

The only properties of f that we use in the rest of the proof are: $f(x) = o(x)$ as $x \to \infty$, and Titchmarsh's theorem (23),

$$\lim_{A \to \infty} \int f^A \mathrm{d}\Pi = 0 \ , \qquad f^A = f \cdot (\chi_{[-A,A]} \circ f) \ .$$

Since $f(x) = o(x)$, we have

$$\sup_{[-B,B]} |f| = o(B) \ , \qquad B \to \infty \ .$$

It follows that there is a function $A = A(B)$ such that $A = o(B)$, $A(\infty) = \infty$, and

$$f = f^{A(B)} \quad \text{on } [-B, B] \; .$$

Then we also have

$$|f \circ \eta_B|, \; |f^{A(B)}| \; \le \; A(B) \quad \text{on } \mathbb{R} \; ,$$

and therefore

$$\int \left| f \circ \eta_B - f^{A(B)} \right| \, \mathrm{d}\Pi \le A(B) \int_{\mathbb{R}\setminus[-B,B]} \mathrm{d}\Pi \; \to \; 0 \; , \qquad B \to \infty \; .$$

□

We leave it to the reader to state relevant results concerning zeros of functions from more general Cartwright–de Branges spaces $B^+(E)$. For example, the key property $\tilde{h} = o(t)$ is valid if

$$\lim_{\delta \to 0} \limsup_{x \to \infty} \frac{\theta(x + \delta x) - \theta(x)}{x} = 0 \; ,$$

where θ is the argument of Θ_E.

Spectral Problems with Mixed Data

4.5 Abstract Hochstadt–Liberman Problem

We will be considering the following problem concerning general meromorphic inner functions. In the next section we will explain its relation to Hochstadt–Liberman's theorem [21].

Let Φ and Ψ be meromorphic inner function and $\Theta = \Psi\Phi$. As usual, $\sigma(\Theta)$ denotes the (point) spectrum of Θ, see Sect. 2.2; recall that $\sigma(\Theta)$ may include ∞. We say that *the data* $[\Psi, \sigma(\Theta)]$ *determine* Θ if for any inner function $\tilde{\Phi}$,

$$\tilde{\Theta} = \Psi\tilde{\Phi}, \quad \sigma(\tilde{\Theta}) = \sigma(\Theta) \quad \Rightarrow \quad \Theta = \tilde{\Theta} \; .$$

Alternatively, we can say that Ψ and $\sigma(\Phi\Psi)$ determine Φ. Given Φ and Ψ, the problem is to decide if this is the case.

The set of Herglotz measures of inner functions $\tilde{\Theta}$ satisfying $\Psi|\tilde{\Theta}$ and $\sigma(\tilde{\Theta}) = \sigma(\Theta)$ is convex, see Sect. 2.2. We will refer to the dimension of this set as the dimension of the set of solutions.

Example 4.12. Suppose Θ is a *finite Blaschke product.* Then

$$[\Psi, \sigma(\Theta)] \text{ determine } \Theta \quad \Leftrightarrow \quad 2 \deg \Psi > \deg \Theta \; .$$

The proof is elementary; it also follows from the results below. As an illustration consider the simplest case $\Theta = b^2$, $\Psi = b$. Then $\sigma(\Theta) = \{0, \infty\}$, and the data $[\Psi, \sigma(\Theta)]$ does not determine Θ. In fact, the set of solutions is one-dimensional; the solutions are given by the formula

$$\tilde{\Phi}(z) = \frac{z - \mathrm{i}a}{z + \mathrm{i}a}\,, \qquad (a > 0)\,.$$

We will state some conditions in terms of the Toeplitz kernels with symbol $U = \bar{\Phi}\Psi$. The rough meaning of these conditions is the following: for the data $[\Psi, \sigma(\Theta)]$ to determine Θ, the known factor Ψ of the inner function has to be "bigger" than the unknown factor Φ.

Proposition 4.13. *If $N^\infty[\bar{\Phi}\Psi] \neq \{0\}$, then the data $[\Psi, \sigma(\Theta)]$ does not determine Θ.*

Proof. Take

$$a \in N^\infty[\bar{\Theta}\Psi^2]\,, \qquad \|a\|_\infty < \frac{1}{2}\,.$$

Then

$$\bar{\Theta}\Psi^2 a = \bar{b}\,,$$

and

$$\bar{\Theta}\Psi^2(a + b) = \bar{a} + \bar{b}\,.$$

Denote

$$g = a + b\,, \qquad f = \Psi g\,,$$

so that

$$\bar{\Theta} f = \bar{f}\,, \qquad \Psi | f\,, \qquad \|f\|_\infty < 1\,.$$

Then the function

$$\tilde{\Theta} = \frac{f + \Theta}{f + 1} \tag{34}$$

is inner:

$$|\tilde{\Theta}|^2 = \frac{(f+\Theta)(\bar{f}+\bar{\Theta})}{(f+1)(\bar{f}+1)} = \frac{(f+\Theta)(\bar{\Theta}f+\bar{\Theta})}{(f+1)(\bar{\Theta}f+1)} = 1\,,$$

and $\Psi | \tilde{\Theta}$. Let us check that $\sigma(\Theta) = \sigma(\tilde{\Theta})$. This is clear for finite eigenvalues, and we also note that $\infty \in \sigma(\Theta)$ iff $\infty \in \sigma(\tilde{\Theta})$ because $\Theta - 1 \in \mathcal{H}^2$ iff

$$\tilde{\Theta} - 1 = \frac{\Theta - 1}{f + 1} \in \mathcal{H}^2\,.$$

□

Here is a partial converse. We write $N^p_\Pi[U]$ for $N^+[U] \cap L^p_\Pi$.

Proposition 4.14. *If $N^p_\Pi[\bar{\Phi}\Psi] = \{0\}$ for some $p < 1$, then $[\Psi, \sigma(\Theta)]$ determine Θ.*

Proof. Suppose $\sigma(\Theta_1) = \sigma(\Theta)$ and $\Psi|\Theta_1$. Then the function

$$f = \frac{\Theta_1 - \Theta}{1 - \Theta_1}$$

is in $\mathcal{H}^p_\Pi \cap C^\omega(\mathbb{R})$ for all $p < 1$ because $(1 - \Theta_1)^{-1}$ has positive real part in $\mathbb{C}_+$ and $\Theta_1 = \Theta$ on $\{\Theta_1 = 1\}$. Observe that

$$\bar{\Theta} f = \bar{\Theta}\frac{\Theta_1 - \Theta}{1 - \Theta_1} = \frac{\Theta_1\bar{\Theta} - 1}{1 - \Theta_1} = \frac{\bar{\Theta} - \bar{\Theta}_1}{\bar{\Theta}_1 - 1} = \bar{f}\ .$$

Since $\Psi|f$, we can define

$$g = \bar{\Psi} f \in \mathcal{H}^p_\Pi \cap C^\omega(\mathbb{R})\ .$$

We have

$$\bar{\Phi}\Psi g = \bar{\Theta}\Psi^2 g = \Psi\bar{\Theta} f = \Psi\bar{f} = \bar{g}\ ,$$

and so $g \in N^p_\Pi[\bar{\Phi}\Psi] = \{0\}$ and $\Theta_1 = \Theta$. □

How big is the gap between the conditions in the above statements? As we will see in Sect. 5.1, the gap is just finite dimensional if the inner function Φ is not very “wild”. Namely, if the argument of Φ has a polynomial growth at infinity, then $N^p_\Pi[\bar{\Phi}\Psi] = \{0\}$ implies $N^\infty[b^n\bar{\Phi}\Psi] = \{0\}$ for some $n < \infty$.

We now demonstrate a different way to state a partial converse of the first statement. We get precisely the converse statement up to a factor which is the ratio of two twin inner functions, see Sect. 3.8.

Proposition 4.15. *If the data $[\Psi, \sigma(\Theta)]$ don't determine Θ, then there are inner functions Θ_1 and J such that $\{\Theta_1 = 1\} = \{J = 1\}$ and*

$$N^\infty[(\bar{\Theta}_1 J)\bar{\Phi}\Psi] \neq 0\ .$$

Proof. Suppose we have $\sigma(\Theta_1) = \sigma(\Theta)$, $\Theta_1 = \Phi_1\Psi$. Then the function $\Phi - \Phi_1$ is in $K^\infty[\Phi\Phi_1]$ and is zero on $\{\Theta_1 = 1\}$. By Proposition 4.4, there is an inner function J such that $J = 1$ exactly on $\{\Theta_1 = 1\}$ and $N^\infty[\bar{\Phi}_1\bar{\Phi}J)] \neq 0$. Finally, we note

$$\bar{\Phi}\bar{\Phi}_1 J = \bar{\Phi}\Psi(\bar{\Theta}_1 J)\ .$$

□

We can apply our results on Toeplitz kernels (Sects. 3 and 5) to obtain various necessary or sufficient conditions in the Hochstadt–Liberman problem. Here is a simple example that extends the original Hochstadt–Liberman theorem, which we will recall in the next subsection.

Corollary 4.16. *Suppose $\Theta = \Psi^2$ and $\infty \notin \sigma(\Theta)$. Then the set of solutions is exactly one-dimensional: $\tilde{\Theta}$ satisfies $\Psi|\tilde{\Theta}$, $\sigma(\tilde{\Theta}) = \sigma(\Theta)$ iff*

$$\exists r \in (-1, 1)\ , \qquad \tilde{\Theta} = \Psi\frac{r + \Psi}{1 + r\Psi}\ . \tag{35}$$

Proof. We have $\Phi = \Psi$, so $N^\infty[\bar\Phi\Psi] \neq 0$ and by the first proposition the dimension is at least 1. On the other hand, the dimension can not be ≥ 2, for otherwise by the last proposition we would have $N^\infty[b\bar\Theta_1 J] \neq 0$ and therefore $N[\bar\Theta_1 J] \neq 0$ for some inner functions Θ_1 and J such that $\{J = 1\} = \{\Theta_1 = 1\}$ and $\sigma(\Theta_1) = \sigma(\Theta)$. By assumption, $\infty \notin \sigma(\Theta_1)$, so and we get a contradiction with the twin function theorem in Sect. 3.8. The formula (35) now follows from the construction (34) in the proof of the first proposition. □

Remark 4.17. One can show that the statement is true even without assumption $\infty \notin \sigma(\Theta)$. Also, one can state the following "one-sided" version (see Remark 3.21 in Sect. 3.8):

Corollary 4.18. *Let $\Theta = \Psi^2$. Then $\tilde\Theta$ satisfies $\Psi|\tilde\Theta$, $\sigma(\tilde\Theta) \subset \sigma(\Theta)$ iff*

$$\exists r \in [-1, 1] , \qquad \tilde\Theta = \Psi \frac{r + \Psi}{1 + r\Psi} .$$

In other words, the (convex) set of all such $\tilde\Theta$'s is the segment $[-\Psi, \Psi]$. Once we know that the dimension is one, the formula follows from the obvious fact that $\pm\Psi$ are extreme points of this set.

4.6 Spectral Theory Interpretation: Hochstadt–Liberman and Khodakovski Theorems

Consider a Schrödinger operator $L = (q, \alpha, \beta)$ on (a, b), where $q \in L^1_{\text{loc}}(a, b)$ and α, β are selfadjoint boundary conditions at a and b respectively; the endpoints can be infinite and/or singular. We assume that L has compact resolvent. As usual, $\sigma(L)$ denotes the spectrum of L.

Suppose $a < c < b$. We will write q_- for the restriction of q to (a, c) and q_+ for the restriction of q to (c, b). We say that the data $(q_-, \alpha, \sigma(L))$ *determines* L if for any other Schrödinger operator $\tilde L = (\tilde q, \tilde\alpha, \tilde\beta)$,

$$q_- = q,\ \alpha = \tilde\alpha,\ \sigma(\tilde L) = \sigma(L) \quad \Rightarrow \quad \tilde q_+ = q_+,\ \tilde\beta = \beta .$$

Let Θ_- denote the Weyl inner function of (q_-, α) computed at c and Θ_+ the Weyl inner function of (q_+, β) computed at c.

Lemma 4.19. $\sigma(L) = \sigma(\Theta_-\Theta_+)$.

Proof. The equation $\Theta_-(\lambda)\Theta_+(\lambda) = 1$ is equivalent to the statement

$$m_+(\lambda) + m_-(\lambda) = 0 \text{ or } m_-(\lambda) = m_+(\lambda) = \infty ,$$

for the corresponding m-functions. The latter means that we have the matching

$$\frac{\dot u_-(c, \lambda)}{u_-(c, \lambda)} = \frac{\dot u_+(c, \lambda)}{u_+(c, \lambda)} ,$$

for any two non-trivial solutions $u_-(\cdot, \lambda)$ and $u_+(\cdot, \lambda)$ of the Schrödinger equation with boundary conditions α and β respectively, which is possible if and only if λ is an eigenvalue of L. □

Corollary 4.20. *$(q_-, \alpha, \sigma(L))$ determine L if the data $(\Theta_-, \sigma(\Theta_-\Theta_+))$ determine Θ_+.*

Here we of course rely on the fundamental uniqueness theorem of Borg and Marchenko [7], [31]: the m–function (and therefore the Weyl inner function) determines both the potential and the boundary condition.

Remark 4.21. We would have an "iff" statement if we considered the problem in some class of canonical systems with a one-to-one correspondence between the systems and inner functions such as the class of Krein's "strings", see [12], [14]. The effective characterization of inner functions of Schrödinger operators is an open problem, so we will use our general results to state only sufficient conditions for Schrödinger operators. To obtain necessary condition one has to use more specific techniques of the Schrödinger operator theory, see [7], [22].

Let us apply the above corollary to the situation described at the end of the last subsection.

Example 4.22. Let L be a Schrödinger operator on $\mathbb{R}$ with compact resolvent and limit point boundary conditions at $\pm\infty$. Suppose the potential $q(x)$ is an even function:

$$q(-x) = q(x)\ , \qquad (x > 0)\ .$$

Then $q|_{\mathbb{R}_-}$ and $\sigma(L)$ determine L.

Proof. By Everitt's theorem [15] (we recall it in the next subsection), all the inner functions $(r + \Psi)/(1 + r + \Psi)$ in (35) with $r \neq 0$ are not Weyl inner functions corresponding to a Schrödinger operator. □

This result is a special case of Khodakovski's theorem [24], where only the equality $q(-x) \leq q(x)$ for $x > 0$ is assumed. The full version of Khodakovski's theorem requires a slightly different approach which we describe in the next subsection. Similarly, from the remark at the end of Sect. 3.5 we derive the following statement.

Let L be as above, and let $\tilde{L}$ be another Schrödinger operator on $(-\infty, b)$, $b \geq 0$. If

$$q = \tilde{q} \quad \text{on } \mathbb{R}_- \qquad \text{and} \qquad \sigma(\tilde{L}) \subset \sigma(L)\ ,$$

then either $\tilde{L} = L$ or $b = 0$ and $\tilde{L}$ is the operator with potential q_- and Dirichlet or Neumann condition at 0.

Example 4.23. Let L be a regular selfadjoint Schrödinger operator on $[a, b]$ with non-Dirichlet boundary conditions α and β at a and b respectively. If $c = (a + b)/2$, then $(q_-, \alpha, \sigma(L))$ determine L.

The statement is also true if one or both boundary conditions are Dirichlet, see next subsection. This is a stronger version of the Hochstadt–Liberman theorem [21], see also [17] which states that if *both* L and $\tilde{L}$ are regular, and $\tilde{q}_- = q_-$, $\tilde{\alpha} = \alpha$, $\sigma(\tilde{L}) = \sigma(L)$, then $\tilde{L} = L$. We *do not* require $\tilde{L}$ to be regular. Also, we can replace $\sigma(\tilde{L}) = \sigma(L)$ with $\sigma(\tilde{L}) \subset \sigma(L)$.

4.7 Everitt's Class of Inner Functions

We need the following well-known fact, see [15]:

Fact 4.24. If $m(z)$ is an m-function of a Schrödinger operator, then

$$m(z) = \mathrm{i}\sqrt{z} + o(1)\ , \qquad (z \to \infty,\ z \in \mathrm{i}\mathbb{R}_+)\ .$$

It follows that if $\Psi(z)$ is a Weyl inner function of a Schrödinger operator, then

$$\Psi(z) = 1 - \frac{2}{\sqrt{z}} + \frac{2}{z} + o\left(\frac{1}{z}\right)\ , \qquad (z \to \infty,\ z \in \mathrm{i}\mathbb{R}_+)\ . \tag{36}$$

This motivates the following definitions. We say that a meromorphic inner function Ψ belongs to the class (Ev) if it satisfies the asymptotic relation (36). (Note though that (36) is by no means a full characterization of Weyl inner functions of Schrödinger operators.)

Definition 4.25. *Let* $\Psi, \Phi \in$ (Ev). *We say that* $[\Psi, \sigma(\Psi\Phi)]$ *determine* Φ in the class *(*Ev*) if*

$$\tilde{\Phi} \in (\mathrm{Ev}), \quad \sigma(\Psi\Phi) = \sigma(\Psi\tilde{\Phi}) \quad \Rightarrow \quad \tilde{\Phi} = \Phi\ .$$

Proposition 4.26. *Let* $\Psi, \Phi \in$ (Ev). *Suppose*

$$\exists p < 1, \quad \dim\ N^p[\bar{\Phi}\Psi] < \infty\ .$$

Furthermore, suppose we have a representation $\bar{\Phi}\Psi = \bar{H}/H$, *where* H *is an outer function such that* $H^{\pm 1} \in C^\omega(\mathbb{R})$, *and*

$$H \neq o\left(\frac{1}{\sqrt{|z|}}\right)\ , \qquad (z \to \infty,\ z \in \mathrm{i}\mathbb{R}_+)\ .$$

Then $(\Psi, \sigma(\Psi\Phi))$ *determine* Φ *in the class (*Ev*).*

Proof. We first argue as in the proof of the second proposition in Sect. 4.5. The function

$$G = \frac{\tilde{\Phi} - \Phi}{1 - \tilde{\Phi}\Psi} \in \mathcal{H}^p_{\Pi} \cap C^\omega(\mathbb{R})$$

satisfies

$$\bar{\Phi}\Psi G = \bar{G}\ . \tag{37}$$

We also derive from (36) that

$$G(z) = o\left(\frac{1}{\sqrt{z}}\right)\ , \qquad (z \to \infty,\ z \in \mathrm{i}\mathbb{R}_+)\ .$$

Since the dimension of the Toeplitz kernel is finite, G has at most finitely many zeros on $\mathbb{R}$ and its inner factor is a finite Blaschke product (if any). Thus we can assume that G is an outer function zero free on $\mathbb{R}$ satisfying (37). But in this case $H = G$, and we have a contradiction. $\square$

Remark 4.27. One can show that the statement is true for all $p \le 2$.

Example 4.28. If $\Phi = \Psi \in$ (Ev), then $(\Psi, \sigma(\Psi\Phi))$ determine Φ in the class (Ev).

Proof. $H = 1 \ne o(|z|^{-1/2})$. □

Example 4.29. If $\Psi = \Theta_D$ and $\Phi = \Theta_N$, see (10), then Ψ and $\sigma(\Psi\Phi)$ determine Φ in (Ev), and if $\Psi = \Theta_N$ and $\Phi = \Theta_D$, then Ψ and the spectrum $\sigma(\Psi\Phi)$ minus any one point determine (in an obvious sense) Φ in the class (Ev). In particular, we have the Hochstadt–Liberman type result for all regular operators with arbitrary boundary conditions.

Proof. Reasoning as in Example 3.19, in the first case we have $H = E_D/E_N$ and so $|H| \sim |z|^{-1/2}$. In the second case, $|H| = |E_N/E_D| \sim |z|^{1/2}$. □

Example 4.30 (Bessel inner functions). This is an extension of the previous example. We want to show that the Hochstadt–Liberman phenomenon occurs not only for regular potentials.

We consider the Bessel inner functions Θ_ν, $\nu \ge -1/2$, see (11). Recall that

$$E_\nu(\lambda) = (1 + \mathrm{i}/2 + \mathrm{i}\nu)G_\nu(\sqrt{\lambda}) + \mathrm{i}F_\nu(\sqrt{\lambda})$$

is a de Branges function of Θ_ν, where $G_\nu(z) = z^{-\nu}J_\nu(z)$ and $F_\nu(z) = zG'_\nu(z)$, see Sect. 2.6. If $\Psi = \Theta_{\nu_1}$ and $\Phi = \Theta_{\nu_2}$, then we have a representation

$$\bar{\Phi}\Psi = \frac{\bar{H}}{H}\,, \qquad H = \frac{E_{\nu_1}}{E_{\nu_2}}\,.$$

Lemma 4.31.

$$\left|\frac{E_{\nu_1}(\lambda)}{E_{\nu_2}(\lambda)}\right| \sim |\lambda|^{\frac{\nu_2-\nu_1}{2}}\,, \qquad \lambda \in \mathrm{i}\mathbb{R}_+,\ \lambda \to \infty\,.$$

Proof. It is known that $|J_\nu(z)| \sim |J_0(z)|$ as $z \to \infty$ in any Stolz angle in $\mathbb{C}_+$. Therefore,

$$|G_\nu(z)| \sim |z^{-\nu}J_0(z)|,$$

and we also have

$$|F_\nu(z)| \sim |G_{\nu-1}(z)| \sim |z^{1-\nu}J_0(z)|\,.$$

(The first relation follows from the identity $zJ'_\nu(z) = zJ_{\nu-1}(z) - \nu J_\nu(z)$, which implies $F_\nu = G_{\nu-1} - 2\nu G_\nu$). □

We can now apply Proposition 4.26. In particular, we get the following result.

Theorem 4.32. *Let L be the Schrödinger operator with potential $q(t) = 2t^{-2}$ on $[0,2]$ and with Dirichlet boundary condition at $t = 2$. Then $q|_{(0,1)}$ and the spectrum $\sigma(L)$ determine L in the class of Schrödinger operators.*

Proof. In our usual notation we have

$$\Psi = \Theta_{3/2}\,, \qquad \bar{\Phi}\Theta_{1/2} = \frac{\bar{F}}{F}, \quad F^{\pm 1} \in H^\infty\,,$$

see Sect. 3.4. Therefore,

$$\bar{\Phi}\Psi = (\bar{\Phi}\Theta_{1/2})\bar{\Theta}_{1/2}\Theta_{3/2} = \frac{\bar{F}}{F}\,\frac{E_{1/2}}{\bar{E}_{1/2}}\,\frac{\bar{E}_{3/2}}{E_{3/2}} = \frac{\bar{H}}{H}\,,$$

where

$$H = \frac{FE_{3/2}}{E_{1/2}}$$

is an outer function such that $H^{\pm 1} \in C^\omega(\mathbb{R})$ and $H(\mathrm{i}y) \neq o(1/\sqrt{y})$ as $y \to +\infty$. We can apply the proposition because the argument of the unimodular function $\bar{\Phi}\Psi$ is bounded, which is a consequence of the well-known asymptotic for the zeros of Bessel's functions. □

Defining Sets

4.8 Defining Sets of Inner Functions

Let $\Phi = \mathrm{e}^{\mathrm{i}\phi}$ be a meromorphic inner function, and let $\Lambda \subset \mathbb{R}$. We say that Λ is a *defining set* for Φ if

$$\tilde{\Phi} = \mathrm{e}^{\mathrm{i}\tilde{\phi}},\ \tilde{\phi} = \phi \text{ on } \Lambda \quad \Rightarrow \quad \Phi \equiv \tilde{\Phi}\,.$$

In this definition we tacitly assume $\phi(\pm\infty) = \pm\infty$. In the "one-sided" case, say if $\phi(-\infty) > -\infty$ and $\phi(+\infty) = +\infty$, one should modify the definition in an obvious way.

One can extend this definition to divisors. For instance, if all points in $\Lambda \subset \sigma(\Phi)$ are double, then the equality $\tilde{\Phi} = \Phi$ on Λ means that the spectral measures the inner functions coincide on Λ.

Let us mention several special cases.

Case 4.33 (Two spectra problem). This corresponds to the case

$$\Lambda = \{\Phi = 1\} \cup \{\Phi = -1\}\,.$$

The meaning of the following statement is that Λ is defining for Φ with deficiency one (in the case $\phi(\pm\infty) = \pm\infty$, to be accurate). Various related statements are of course well-known, see e.g. [7].

Let Φ be a meromorphic inner function. Then a meromorphic inner function $\tilde{\Phi}$ satisfies $\{\tilde{\Phi} = 1\} = \{\Phi = 1\}$ and $\{\tilde{\Phi} = -1\} = \{\Phi = -1\}$ iff

$$\tilde{\Phi} = \frac{\Phi - c}{1 - c\Phi}\,, \qquad c \in (-1, 1)\,. \tag{38}$$

The easiest way to see this is use Krein's shift construction: since

$$\Re\left[\frac{1}{\pi \mathrm{i}}\log\frac{\tilde{\Phi}+1}{\tilde{\Phi}-1}\right]=\chi_e \quad \text{on } \mathbb{R}\,,$$

where $e=\{\Im\Phi>0\}$, we have

$$\frac{1}{\pi \mathrm{i}}\log\frac{\tilde{\Phi}+1}{\tilde{\Phi}-1}=\mathcal{S}\chi_e+\text{const}\,.$$

This argument also shows that *given any two intertwining discrete sets* $\Lambda_\pm$ *of real numbers there is a meromorphic inner function* Φ *such that*

$$\{\Phi=\pm 1\}=\Lambda_\pm\,.$$

Let us also mention that the statement (38) can be derived from the twin inner function theorem, see Sect. 3.8. For instance, suppose $I:=\tilde{\Phi}\Phi$ has no point mass at infinity. We want to show that $\tilde{\Phi}-\Phi=c(1-I)$. It is enough to check that the dimension of the set of functions $F\in K_I^\infty$ vanishing on $\{I=1\}$ is at most one. (Obviously, both $\tilde{\Phi}-\Phi$ and $1-I$ belong to this set.) If not, we would have $\dim\ N^\infty[\bar{I}J]\geq 2$ for some J vanishing on $\{I=1\}$. But then $N^\infty[b\bar{I}J]\neq 0$, and $N[\bar{I}J]\neq 0$, which is impossible by the twin inner function theorem.

Case 4.34 (General mixed data spectral problem). The Hochstadt–Liberman problem for inner functions that we discussed above can be viewed as a special case of the defining sets problem. It is easy to see that if (assuming $\arg\Theta(\pm\infty)=\pm\infty$) $\Theta=\Psi\Phi$ and $\Lambda=\sigma(\Theta)$, then

$$(\Psi,\sigma(\Theta)) \text{ determine } \Theta \quad\Leftrightarrow\quad \Lambda \text{ is defining for } \Phi\,.$$

This can be generalized in the following way. Let $\Theta=\Psi\Phi$ be a given meromorphic inner function and let $\{\lambda_n\}$ be the set of its eigenvalues numbered in the increasing order. Given $M\subset\mathbb{Z}$ we denote

$$\sigma_M(\Theta)=\{\lambda_n:\ n\in M\}\,.$$

The question is whether the factor Ψ and the partial spectrum $\sigma_M(\Theta)$ determine Θ, i.e. whether

$$\tilde{\Theta}=\Psi\tilde{\Phi},\quad \tilde{\lambda}_n=\lambda_n\ (n\in M)\qquad\Rightarrow\qquad \tilde{\Theta}\equiv\Theta\,.$$

Once again, this is equivalent (assuming $\phi(\pm\infty)=\pm\infty$) to saying that $\Lambda=\sigma_M(\Theta)$ is a defining set for Φ. The spectral theory meaning was explained in Sect. 4.6 (but now we consider eigenvalues from different spectra), and the partial spectral problem for Schrödinger operators and Jacobi matrices appeared in several publications, e.g. [17], [18].

Case 4.35 (A version for spectral measures). Given a meromorphic inner function Θ and a factor $\Psi|\Theta$, and also given a part of the spectrum $\Lambda = \sigma_M(\Theta)$, the question is whether there is another inner function $\tilde{\Theta} \neq \Theta$ such that $\Psi|\tilde{\Theta}$ and the spectral measures $\mu = \mu_\Theta$ and $\tilde{\mu} = \mu_{\tilde{\Theta}}$ coincide on Λ:

$$\tilde{\lambda}_n = \lambda_n, \quad \tilde{\mu}\{\lambda_n\} = \tilde{\mu}\{\lambda_n\}, \qquad (n \in M) .$$

Claim. If $\Theta = \Psi\Phi$, then Ψ and the spectral measure on $\Lambda = \sigma_M(\Theta)$ determine Θ iff the divisor $2\chi_\Lambda$ is defining for Φ.

Indeed, if $\tilde{\Theta} = \Psi\tilde{\Phi}$, and

$$\arg\tilde{\Theta}(\lambda_n) = \arg\tilde{\Theta}(\lambda_n) = 2\pi n , \qquad (n \in M) ,$$

then

$$\arg\tilde{\Phi} = \arg\Phi \quad \text{on } \Lambda .$$

The relation

$$\mu\{\lambda\} = \tilde{\mu}\{\lambda\} , \qquad \lambda \in \Lambda$$

then implies, see (7), $\tilde{\Theta}'(\lambda) = \Theta'(\lambda)$, so

$$\Psi'(\lambda)\tilde{\Phi}(\lambda) + \Psi(\lambda)\tilde{\Phi}'(\lambda) = \Psi'(\lambda)\Phi(\lambda) + \Psi(\lambda)\Phi'(\lambda) , \qquad (\lambda \in \Lambda) ,$$

and

$$(\arg\tilde{\Phi})' = (\arg\Phi)' \quad \text{on } \Lambda .$$

Again, the spectral theory interpretation is the same as above: we know some part of a differential operator and some part of its spectral measure and we want to know if this information determines the operator uniquely.

As usual we can consider the problem in a restricted class of inner functions. Here is the simplest example.

Example 4.36. Let $\Theta = \Psi\Phi$ be a finite Blaschke product. Then Ψ and $\Lambda \subset \sigma(\Theta)$ determine Θ iff $\#\Lambda > 2\deg\ \Phi$ in the class of Blaschke products of a fixed degree. Similarly, Ψ and the spectral measure on Λ determine Θ iff $\#\Lambda > \deg\ \Phi$. This extends in an obvious way to the cases where only Φ or Ψ has a finite degree. These facts follow for instance from the statements in the next section, also cf. [18].

4.9 Relation to Uniqueness Sets

Proposition 4.37. *Λ is not defining for Φ if there is a non-constant function $G \in K_\Phi^\infty$ such that*

$$G = \bar{G} \ \text{on } \Lambda . \tag{39}$$

Proof. We can assume $\|G\|_\infty < 1$. Define $F \in H^\infty$ by the equation $\bar{\Phi}G = \bar{F}$ on $\mathbb{R}$, and consider

$$\tilde{\Phi} = \frac{\Phi + F}{1 + G} .$$

Then $\tilde{\Phi}$ is an inner function because it is in $\mathcal{N}^+$ and

$$|\Phi + F| = |\Phi + \Phi\bar{G}| = |1 + G| \quad \text{on } \mathbb{R} .$$

Also, $\tilde{\Phi} \neq \Phi$ because otherwise we would have $F = G\Phi$, which together with $F = \Phi\bar{G}$ implies $G = \bar{G}$, so $G = \text{const}$. Finally, we have

$$\tilde{\Phi} = \Phi\frac{1 + \bar{\Phi}F}{1 + G} = \Phi\frac{1 + \bar{G}}{1 + G} = \Phi \quad \text{on } \Lambda ,$$

and since

$$\| \arg\ \tilde{\Phi} - \arg\ \Phi\|_{L^\infty(\mathbb{R})} < 2\pi$$

by construction, we get $\arg\ \tilde{\Phi} = \arg\ \Phi$ on Λ. □

Remark 4.38. The condition (39) is very close to the condition that Λ is a not a uniqueness set for $K^\infty[\Phi^2]$. The precise relation between the two statements is an interesting question, which we will not discuss here. We only mention that if $p \in (1, \infty)$, then

$$\exists G \in K^p[\Phi] , \quad G \not\equiv \text{const} , \quad G = \bar{G} \text{ on } \Lambda ,$$

iff

$$\exists F \in K^p[\Phi^2] , \qquad F \not\equiv 0 , \quad F = 0 \text{ on } \Lambda .$$

The above proposition gives a necessary condition for a set Λ to be defining for Φ. To get sufficient conditions one can use the following obvious observation.

Lemma 4.39. *If $\tilde{\Phi} = \Phi$ on Λ and $F = \tilde{\Phi} - \Phi$, then*

$$F \in K^\infty[\tilde{\Phi}\Phi] , \qquad F = 0 \text{ on } \Lambda .$$

If we also have $\arg\ \tilde{\Phi} = \arg\ \Phi$ on Λ (as in the definition of defining sets), then we can estimate the argument of $\tilde{\Phi}\Phi$ in terms of the data (Φ, Λ), so we can apply our results concerning uniqueness sets.

4.10 Defining Sets of Regular Operators. Horváth Theorem.

We now consider the defining sets problem in some restricted classes of inner functions. We will use the spectral theory language. For $r \geq 1$ let $\text{Schr}(L^r, D)$ denote the class of selfadjoint Schrödinger operators on $[0, 1]$ with an L^r potential and Dirichlet boundary condition at 0.

We say that $\Lambda \subset \mathbb{R}$ is a *defining set for the class* $\mathrm{Schr}(L^r, D)$ if for any two operators in $\mathrm{Schr}(L^r, D)$ with potentials q and $\tilde{q}$, the equality $\tilde{\Theta} = \Theta$ on Λ implies $\tilde{q} \equiv q$, where $\tilde{\Theta}$ and Θ are the corresponding Weyl inner functions.

We have a similar definition for the classes $\mathrm{Schr}(L^r, N)$ of Schrödinger operators with Neumann boundary condition at 0.

Let Θ_D denote the standard inner function (10), i.e. the Weyl inner function in the case $q \equiv 0$. From Lemma 4.39 we immediately conclude that Λ *is defining in the class* $\mathrm{Schr}(L^1, D)$ *if* Λ *is a uniqueness set of* $K^\infty[\Theta_D^2]$.

This sufficient condition is not optimal because for regular operators, the function $\tilde{\Phi} - \Phi$ (see the statement of Lemma 4.39) has some extra smoothness at infinity as follows from the standard asymptotic formulae (see the end of the section), which are getting more precise if we require more regularity of the potential, in particular if we consider the case $q \in L^r$ with $r > 1$.

In an interesting paper [22], Horváth gives a complete description of defining sets in terms of uniqueness sets of certain model spaces (or, equivalently, in terms of the completeness problem for exponential functions). The description involves the spaces $\mathcal{F}L^r \equiv \mathcal{F}L^r(-2, 2)$, where $\mathcal{F}$ stands for the classical Fourier transform (1). Recall that

$$PW_2 = \mathcal{F}L^2 \subset \mathcal{F}L^1 \subset \mathrm{Cart}_2 \cap \mathrm{L}^\infty(\mathbb{R}) .$$

Here is a selection of Horváth's results. We use the following notation: $\sqrt{\Lambda} = \{z : z^2 \in \Lambda\}$, and $\sqrt{\Lambda} \cup \{*, *\}$ means $\sqrt{\Lambda}$ plus any two points.

(i) Λ *is defining in the class* $\mathrm{Schr}(L^r, D)$ *iff* $\sqrt{\Lambda} \cup \{*, *\}$ *is a uniqueness set of* $\mathcal{F}L^r$*;*
(ii) Λ *is defining in* $\mathrm{Schr}(L^r, N)$ *if* $\sqrt{\Lambda}$ *is not a zero set of* $\mathcal{F}L^r$*.*

(In the second case, the "only if" part of Horváth's theorem comes with some additional condition.)

Let us explain how to prove the "if" parts of these statements using the methods of this paper. We prove for example (ii).

Proposition 4.40. Λ *is defining in the class* $\mathrm{Schr}(L^2, D)$ *if* $\sqrt{\Lambda} \cup \{*, *\}$ *is a uniqueness set of* PW_2*.*

Proof. Let $q, \tilde{q} \in L^2(0, 1)$. Without loss of generality we will assume that the corresponding Schrödinger operators with boundary conditions (D) at 0 and (N) at 1 are positive. Otherwise, we simply add a large positive constant a to both potentials, and using the transformation

$$F(z) \mapsto F(\sqrt{z^2 + a^2})$$

for even entire functions we observe that $\sqrt{\Lambda}$ is a uniqueness set iff $\sqrt{\Lambda + a}$ is.

Let Θ^* and $\tilde{\Theta}^*(z)$ be the square root transforms of Θ and $\tilde{\Theta}$, the Weyl functions taken with sign minus, see Sect. 2.8. From the standard asymptotic formula for solutions of a regular Schrödinger equation we obtain

$$\frac{\Theta^*}{S^2} = \frac{\bar{H}}{H} \text{ on } \mathbb{R} , \qquad H^{\pm 1} \in H^\infty , \tag{40}$$

and

$$x[\Theta^*(x) - \tilde{\Theta}^*(x)] \in L^2(\mathbb{R}) . \tag{41}$$

(For convenience we reproduce the standard argument at the end of the proof.)

If $\tilde{\Theta} = \Theta$ on Λ, then since $\tilde{\Theta}^*(0) = \Theta^*(0)$, we have

$$\Theta^* = \tilde{\Theta}^* \quad \text{on } \{0\} \cup \sqrt{\Lambda} ,$$

where we regard Θ^* and $\tilde{\Theta}^*$ as meromorphic functions in the whole plane. By (41),

$$(z-1)(\Theta^* - \tilde{\Theta}^*) \in K[\Theta^* \tilde{\Theta}^*] ,$$

so $\sqrt{\Lambda} \cup \{0,1\}$ is a zero set of some $K[\Theta^* \tilde{\Theta}^*]$ function, and therefore by (40) a zero set of some function in $K[S^4]$ or PW_2. (For zeros in $\mathbb{C}_-$ we can use the argument with dual reproducing kernels as in Sect. 4.1.) □

Proof (of (40)–(41)*).* If $s > 0$, then the solution $u_s(t)$ of the IVP

$$-\ddot{u} + qu = s^2 u , \qquad u(0) = 0 , \quad \dot{u}(0) = 1 ,$$

satisfies the integral equation

$$u_s(x) = \sin sx + \frac{1}{s} \int_0^x \cos s(x-t) \; q(t) \; u_s(t) \; \mathrm{d}t .$$

Iterating, we have

$$u_s(1) = \sin s + \frac{F(s)}{s} + \frac{R(s)}{s^2} ,$$

where

$$F(s) = \int_0^1 \cos s(1-t) \; \sin st \; q(t) \; \mathrm{d}t ,$$

and

$$R(s) = \int_0^1 \cos s(1-x) \; q(x) \; \mathrm{d}x \int_0^x \cos s(x-t) \; q(t) \; u_s(t) \; \mathrm{d}t .$$

We have an elementary a priori bound

$$|u_s(t)| \le C , \qquad (s > 0, \; t \in [0,1]) ,$$

so

$$\forall s, \quad |R(s)| \le \text{const} .$$

On the other hand, F is basically the Fourier transform of a function on $(-1,1)$, and

$$q \in L^2 \quad \Rightarrow \quad F \in L^2(\mathbb{R}) .$$

We also get the corresponding estimates of $\dot{u}_s(1)$. The resulting estimates of Θ imply both statements. □

5 Beurling–Malliavin Theory

Multiplier Theorems

5.1 Tempered Inner Functions

A meromorphic inner function $\Theta = e^{i\Theta}$ is called *tempered* if Θ' has at most polynomial growth at $\pm\infty$:

$$\exists N, \quad \Theta'(x) = O\left(|x|^N\right), \quad x \to \infty .$$

Theorem 5.1. *Suppose Θ is a tempered inner function. Then for any meromorphic inner function J and any $p > 0$,*

$$N^p[\bar{\Theta}J] \neq 0 \quad \Rightarrow \quad \exists n,\ N^\infty[\bar{b}^n\bar{\Theta}J] \neq 0 .$$

Note that the opposite is trivial: if $q > p$ then $N^q[\bar{\Theta}J] \neq 0$ implies $N^p[\bar{b}^n\bar{\Theta}J] \neq 0$ with $n = n(p,q)$. Questions of this type were studied by Dyakonov [13] who was the first to observe the analogy with the Beurling–Malliavin multiplier theorem.

The proof for $p = 2$ is elementary: if $F \in N[\bar{\Theta}J]$, then $JF \in K_\Theta$ and by (9) and (7),

$$\sum_{\lambda \in \sigma(\Theta)} \frac{|F(\lambda)|^2}{|\Theta'(\lambda)|} \asymp \|F\|^2 .$$

Thus $|F(\lambda)| \lesssim |\Theta'(\lambda)|$, and this is true for all $\lambda \in \mathbb{R}$ because we can replace Θ with $e^{-i\alpha}\Theta$. It follows that $(z+i)^{-n}F(z) \in N^\infty[\bar{b}^n\bar{\Theta}J]$.

We will derive the theorem from the following special case of Carleson's type embedding theorem of Treil and Volberg [40]. For a given meromorphic inner function Θ denote

$$d(x) = \operatorname{dist}\{x, \{|\Theta| = 0.5\}\} , \qquad (x \in \mathbb{R}) .$$

Claim. The measure $\nu_x = d(x)\delta_x$ is a Carleson measure for K^p_Θ, i.e.

$$K^p_\Theta \subset L^p(\nu) ,$$

where the norm of the embedding depends only on p.

In other words, if $F \in K^p_\Theta$, then

$$d(x)\ |F(x)|^p \leq \text{const} , \qquad (x \in \mathbb{R}) . \tag{42}$$

Lemma 5.2. *If Θ is tempered, then there is an N such that*

$$\operatorname{dist}(x, \{|\Phi| = 0.5\} \gtrsim (1+|x|)^{-N} .$$

Proof. We can only consider the case of Blaschke products. If

$$\Theta = B_\Lambda = \prod \epsilon_\lambda \frac{z-\lambda}{z-\bar{\lambda}} \,,$$

then we have

$$\Theta'(x) = \sum \frac{2\Im\lambda}{|x-\lambda|^2} \tag{43}$$

and

$$-\log|\Theta(z)| \asymp \sum \frac{\Im\lambda \times \Im z}{|z-\bar{\lambda}|^2} \,. \tag{44}$$

Indeed,

$$\begin{aligned} -\log|\Theta(z)|^2 &= \sum \log\left|\frac{z-\bar{\lambda}}{z-\lambda}\right|^2 \\ &\asymp \sum \left[1 - \frac{|z-\lambda|^2}{|z-\bar{\lambda}|^2}\right] \qquad \text{(see below)} \\ &= \sum \frac{(z-\bar{z})(\lambda-\bar{\lambda})}{|z-\bar{\lambda}|^2} \end{aligned}$$

We want to show that if $z = x + \mathrm{i}y$ and $y \ll |x|^{-N}$, then (44)< const. For each x consider the Stolz sector of some fixed angle at x of height x^{-N} and observe that this sector does not contain any λ, for otherwise, the corresponding term in (43) would be of the order $1/\Im\lambda \geq x^N$. This justifies the "see below" item, and makes the estimate of (44) in terms of (43) obvious. □

Proof (Theorem 5.1). Suppose $N^p[\bar{\Theta}J] \neq 0$, so

$$\bar{\Theta}JF = \bar{G} \,, \qquad F, G \in \mathcal{H}^p \cap C^\omega(\mathbb{R}) \,.$$

We have

$$JF \in K^p_\Theta \,,$$

so by the lemma and by (42) we have

$$|F(x)| \lesssim 1 + |x|^N \,,$$

for all $x \in \mathbb{R}$ and some N. It follows that $(z+\mathrm{i})^{-N}F(z) \in N^\infty[\bar{b}^N\bar{\Theta}J]$. □

Corollary 5.3. *Let $U = \bar{\Theta}J = \mathrm{e}^{\mathrm{i}\gamma}$ and let Θ be tempered. If γ is the sum of a bounded and a decreasing functions, then $N^\infty[\bar{b}^nU] \neq 0$ for some n.*

Note that in the case of a general bounded γ, we can not multiply down to $\mathcal{H}^\infty$ elements of $N[U]$ even by using factors like $\bar{S}$.

Also note that in the statement of the theorem one can give explicit bounds on n in terms of the growth of $|\Theta'(x)|$. For example, if $U = \bar{\Theta}J$ and $\Theta' \leq 1$, then $N[U] \subset N^\infty[U]$.

5.2 Beurling–Malliavin Multiplier Theorem

Theorem 5.4. *Suppose Θ is a meromorphic inner function satisfying $|\Theta'| \le$ const. Then for any meromorphic inner function J, we have*

$$N^+[\bar{\Theta}J] \neq 0 \quad \Rightarrow \quad \forall\epsilon,\ N^\infty[\bar{S}^\epsilon\bar{\Theta}J] \neq 0\ .$$

This theorem follows from the Beurling–Malliavin multiplier theorem [4]: if W is an outer function, then

$$z^{-1}\log W(z) \in \mathcal{D}(\mathbb{C}_+) \quad \Rightarrow \quad W \in (\mathrm{BM})\ . \tag{45}$$

Here $\mathcal{D}(\mathbb{C}_+)$ is the notation for the usual Dirichlet space in the halfplane, and by definition, W is a *Beurling–Malliavin multiplier*, or $W \in (\mathrm{BM})$, if

$$\forall\epsilon > 0,\ \exists G \in K[S^\epsilon], \qquad WG \in L^2(\mathbb{R})\ .$$

Note that if $|W| \le |W_1|$ and $W_1 \in (\mathrm{BM})$, then $W \in (\mathrm{BM})$.

Lemma 5.5. *If $W \in C^\omega(\mathbb{R})$, $|W| \ge 1$, and $(\arg W)' \le$ const on $\mathbb{R}$, then $W \in (\mathrm{BM})$.*

Proof. We will use some ideas from the proof of Theorem 64 in [12]. We can assume $|W(0)| = 1$. Otherwise, multiply W by $(z + \mathrm{i})$ to get $W(\infty) = \infty$. In this case there's a global minimum, which we can take for 0.

Denote

$$z^{-1}\log W(z) = u(z) + \mathrm{i}v(z)\ ,$$

where u and v are real-valued functions. Then we have

$$x^{-1}u(x) \in L^1(\mathbb{R})\ , \qquad x^{-1}u(x) \ge 0 \text{ on } \mathbb{R}\ . \tag{46}$$

Since $\arg W \in \tilde{L}^1_\Pi$ and $(\arg W)' \le$ const on $\mathbb{R}$, by Lemma 4.9 we have

$$\arg W(x) = o(|x|)\ , \qquad x \in \mathbb{R},\ x \to \infty\ , \tag{47}$$

and it follows that v is a bounded function in $\mathbb{C}_+$. For $r > 0$ let $D(r)$ denote the semidisc $\{|z| < r\} \cap \mathbb{C}_+$. We have

$$\|u + \mathrm{i}v\|^2_{\mathcal{D}} = \lim_{r\to\infty} \int_{\partial D(r)} u\mathrm{d}v\ ,$$

and

$$\int_{\partial D(r)} u\mathrm{d}v = \int_{-r}^{r} uv'\mathrm{d}x - uv\Big|_{-r}^{r} + rI'(r)\ , \qquad I(r) := \frac{1}{2}\int_0^\pi v^2\left(r\mathrm{e}^{\mathrm{i}\theta}\right)\mathrm{d}\theta\ .$$

By (46) and (47), the integrals $\int uv'\mathrm{d}x$ are uniformly bounded from above:

$$\int_{-r}^{r} uv'\mathrm{d}x = \int_{-r}^{r} \frac{u(x)}{x}(\arg W)'(x)\mathrm{d}x - \int_{-r}^{r} \frac{u(x)}{x}\frac{\arg W(x)}{x}\mathrm{d}x < \text{const} .$$

It remains to show that

$$\liminf_{r\to\infty} A(r) < \infty , \qquad A(r) := rI'(r) - uv\Big|_{-r}^{r} .$$

Suppose $A(r) \geq 1$ for all $r \gg 1$. Then since v is bounded, we have

$$I'(r) \geq \frac{1}{r} - \text{const}\frac{u(r)+u(-r)}{r} .$$

By (46), this contradicts the uniform boundedness of $I(r)$. □

Corollary 5.6. *If* $W \in K_\Theta^+$ *and* $(\arg\Theta)' \leq \text{const}$*, then* $W \in (\text{BM})$.

Proof. We have $W\bar\Theta = \bar H$ for some $H \in \mathcal{N}^+$. Define

$$W_1 = WH + \Theta .$$

Clearly, $W_1 \in \mathcal{N}^+$, and since

$$\bar\Theta^2 W_1 = \bar\Theta W \bar\Theta H + \bar\Theta = \bar H \bar W + \bar\Theta = \bar W_1 ,$$

we have $W_1 \in K^+[\Theta^2]$. Notice that

$$|W_1| = |W\bar W\Theta + \Theta| = 1 + |W|^2 \geq 1 .$$

Also, $|W| \leq |W_1|$. Since $(\arg\Theta)' \leq \text{const}$, from the equation $\bar\Theta^2 W_1 = \bar W_1 \bar\Phi$, where Φ is an inner function, we obtain $(\arg W_1)' \leq \text{const}$. By the previous lemma, $W_1 \in (\text{BM})$, and therefore $W \in (\text{BM})$. □

Proof (Theorem 5.4). Take an outer function $W \in N^+[\bar\Theta J]$. Then $W \in K_\Theta^+$ and by the last corollary, $W \in (\text{BM})$, and therefore $WG \in \mathcal{H}^2$ for some $G \in N^+[\bar S^\epsilon]$. It then follows that

$$WG \in N^+[\bar S^\epsilon \bar\Theta J] \cap \mathcal{H}^2 = N[\bar S^\epsilon \bar\Theta J] .$$

It remains to multiply down to $\mathcal{H}^\infty$, which is possible by Theorem 5.1. □

$\mathcal{N}^+$–Part of the Beurling–Malliavin Theory

In this part of the section we will assume

$$\gamma' \geq -\text{const} . \tag{48}$$

We'll give a metric criterion for (non-)triviality of the Toeplitz kernel $N^+[\mathrm{e}^{\mathrm{i}\gamma}]$ up to a gap $S^{\pm\epsilon}$. Recall the basic criterion: $N^+[\mathrm{e}^{\mathrm{i}\gamma}] \neq 0$ iff

$$\gamma = -\alpha + \tilde h , \tag{49}$$

for some increasing function $\alpha \in C^\omega(\mathbb{R})$ and some $h \in L^1_\Pi$. As usual we denote $U = \mathrm{e}^{\mathrm{i}\gamma}$.

Lemma 5.7. *Suppose* $\gamma' \geq -\text{const}$. *Then* $\forall \epsilon > 0$, $N^+[US^\epsilon] = 0$ *unless* $\gamma(\mp\infty) = \pm\infty$.

Proof. If $N^+[US^\epsilon] \neq 0$, then by (49) $\gamma + \epsilon x + \alpha = \tilde{h}$, so $(\tilde{h})' \geq -\text{const}$ and of course $\tilde{h} \in L_\Pi^{o(1,\infty)}$. By Lemma 4.9 it then follows that $\tilde{h}(x) = o(x)$ as $x \to \pm\infty$, so $\gamma + \epsilon x + \alpha = o(x)$, which is possible only if $\gamma(\mp\infty) = \pm\infty$. □

5.3 Beurling–Malliavin Intervals

Suppose a continuous function $\gamma : \mathbb{R} \to \mathbb{R}$ satisfies

$$\gamma(-\infty) = +\infty\ , \qquad \gamma(+\infty) = -\infty\ . \tag{50}$$

The family $\mathcal{BM}(\gamma)$ is defined as the collection of the components of the open set $\{\gamma^\star \neq \gamma\}$, where

$$\gamma^\star(x) = \max_{[x,+\infty]} \gamma\ .$$

For an interval $l = [a, b] \subset \mathbb{R}_+$ or $\subset \mathbb{R}_-$ we write $|l|$ for the Euclidean length, and $\delta(l)$ for the distance from the origin. A family of finite disjoint intervals $\{l\}$ is called *long* if

$$\sum_{\delta(l)\geq 1} \frac{|l|^2}{\delta(l)^2} = \infty\ .$$

Otherwise, we call the family *short*.

Theorem 5.8. *Suppose* $\gamma' > -\text{const}$.

(i) If $\gamma \notin (50)$, *or if* $\gamma \in (50)$ *but the family* $\mathcal{BM}(\gamma)$ *is long, then*

$$\forall \epsilon > 0, \quad N^+[S^\epsilon U] = 0\ .$$

(ii) If $\gamma \in (50)$ *and* $\mathcal{BM}(\gamma)$ *is short, then*

$$\forall \epsilon > 0, \quad N^+[\bar{S}^\epsilon U] \neq 0\ .$$

The first statement corresponds to the "second Beurling–Malliavin theorem" [5], and statement (ii) to the so called "little multiplier theorem", see [25], [19].

5.4 Second Beurling–Malliavin Theorem

The first part of Theorem 5.8 follows from a more general fact; we don't need to assume (48). For an interval $l \subset \mathbb{R}$ we denote

$$\Delta_l^*[\gamma] = \inf_{l''} \gamma - \sup_{l'} \gamma\ ,$$

where l' and l'' are the left and the right adjacent intervals of length $|l|$.

Theorem 5.9. *If* $\exists c > 0$ *and a long family of intervals* $\{l\}$ *such that*

$$\Delta_l^*[\gamma] \geq c|l| , \tag{51}$$

then $N^+[U] = 0$.

A simple standard argument shows that we can assume without loss of generality that all intervals satisfy the inequality $10|l| < \delta(l)$, and that the multiplicity of the covering $\{10l\}$ is finite. (The interval $10l$ is concentric with l and has length $10|l|$.)

The idea of the proof is quite simple. According to the basic criterion (49) we have to exclude the possibility

$$\gamma + \alpha = \tilde{h} , \qquad \alpha \uparrow, \ h \in L^1_\Pi .$$

Since α is increasing we have

$$\Delta_l^*[\tilde{h}] \gtrsim |l| .$$

Suppose we can localize this estimate to each function $\tilde{h}_l$, where h_l is the restriction of h to the interval $10l$. Choosing $A \asymp |l|$ and applying the weak type inequality, we have

$$\frac{|l|}{\delta(l)^2} \lesssim \Pi\{|\tilde{h}_l| > A\} \lesssim \frac{\|h_l\|_\Pi}{A} , \tag{52}$$

so

$$\frac{|l|^2}{\delta(l)^2} \lesssim \|h_l\|_\Pi . \tag{53}$$

Summing up over l's we arrive at a contradiction:

$$\infty = \sum \frac{|l|^2}{\delta(l)^2} \lesssim \sum \|h_l\|_\Pi \lesssim \|h\|_\Pi < \infty .$$

Proof (Theorem 5.9). For an interval l we denote by Q_l its Carleson square:

$$Q_l = \{z : x \in l, \ |l| < y < 2|l|\} .$$

Also, denote

$$H(z) = \int_{\mathbb{R}} \frac{h^-(t)\mathrm{d}t}{(t-z)^2} , \qquad (z \in \mathbb{C}_+) ,$$

where as usual $h^- = \max\{0, -h\}$. We claim that if the estimate (53) does not hold for some interval l in our family, then

$$|H| \gtrsim 1 \text{ on } Q_l . \tag{54}$$

To see this we observe that the argument (52) is valid unless there is an interval l_1, $l \subset l_1 \subset l \cup l' \cup l''$, such that

$$\Delta_{l_1}\tilde{f} \geq (c/2)|l| \,, \qquad f := h - h_l \,.$$

Let's assume (for simplicity of notation) $l_1 = l$, so $\Delta\tilde{f} \equiv \Delta_l\tilde{f} \gtrsim l$. Represent $f = f^+ - f^-$, $f^\pm \geq 0$. The functions $\tilde{f}^\pm$ are decreasing on l:

$$\tilde{f}'_\pm(x) = -\frac{1}{\pi}\int_{\mathbb{R}\setminus(10l)} \frac{f^\pm(t)\mathrm{d}t}{(t-x)^2} > 0 \,, \qquad (x \in l) \,.$$

It follows that $-\Delta\tilde{f}^- \gtrsim |l|$, and so there is a point $x_* \in l$ such that

$$\frac{1}{\pi}\int \frac{f^-(t)\mathrm{d}t}{(t-x_*)^2} = -\tilde{f}'_-(x_*) = -\frac{\Delta\tilde{f}^-}{|l|} \gtrsim 1 \,.$$

If $z \in Q_l$, then

$$\left|\int \frac{f^-(t)\mathrm{d}t}{(t-z)^2}\right| \geq \int \Re\left[\frac{1}{(t-z)^2}\right] f^-(t)\mathrm{d}t \asymp \int \frac{f^-(t)\mathrm{d}t}{(t-x_*)^2} \gtrsim 1 \,.$$

On the other hand, if $z \in Q_l$ and if (53) is not true, then

$$\left|\int \frac{h_l^-(t)\mathrm{d}t}{(t-z)^2}\right| \;\lesssim\; \frac{1}{|l|^2}\int_{(10l)} |h| \;\asymp\; \frac{\delta(l)^2}{|l|^2}\int_{(10l)} |h|\mathrm{d}\Pi \;\ll\; \frac{\delta(l)^2}{|l|^2}\frac{|l|^2}{\delta(l)^2} \;=\; 1 \,,$$

and we get

$$|H(z)| = \left|\int \frac{f^-(t)+h_l^-(t)}{(t-z)^2}\mathrm{d}t\right| \geq \left|\int \frac{f^-(t)\mathrm{d}t}{(t-z)^2}\right| - \left|\int \frac{h_l^-(t)\mathrm{d}t}{(t-z)^2}\right| \gtrsim 1 \,.$$

To finish the proof of the theorem it remains to show that

$$\sum_{l\in(*)} \frac{|l|^2}{\delta(l)^2} < \infty \,,$$

where we write $l \in (*)$ if (54) holds for l. Denote $\psi = \sum_{l\in(*)} |l|\chi_l$, so

$$\sum_{l\in(*)} \frac{|l|^2}{\delta(l)^2} \asymp \int \frac{\psi(t)\mathrm{d}t}{1+t^2} \,.$$

Then we have

$$\int \frac{\psi(t)}{1+t^2}\mathrm{d}t \lesssim \int_1^\infty \frac{\mathrm{d}A}{A^3}\int_{-A}^{A} \psi(t)\mathrm{d}t \,.$$

Fix $C \gg 1$ such that

$$\int_{|t|\geq C} \frac{h^-(t)\mathrm{d}t}{1+t^2} \ll 1 \,.$$

We claim that

$$\int_{-A}^{A} \psi(t)\mathrm{d}t \lesssim \int_{-CA}^{CA} h^-(t)\mathrm{d}t \ ,$$

so we have

$$\int \frac{\psi(t)}{1+t^2}\mathrm{d}t \lesssim \int_1^\infty \frac{\mathrm{d}A}{A^3} \int_{-CA}^{CA} h^-(t)\mathrm{d}t \lesssim \|h\|_\Pi$$

(and we are done). To prove the claim, fix A and consider the 2D Hilbert transform

$$H_A(z) = \int_{-CA}^{CA} \frac{h^-(t)\mathrm{d}t}{(t-z)^2} \ .$$

If $l \subset (-A, A)$ and $l \in (*)$, then

$$|H_A(z)| \asymp |H(z)| \gtrsim 1 \ , \qquad z \in Q_l \ ,$$

by the choice of C. Applying the weak–L^1 estimate for the Hilbert transform, we get

$$\int_{-A}^{A} \psi(t)\mathrm{d}t \lesssim \mathrm{Area}(|H_A| \gtrsim 1) \lesssim \int_{-CA}^{CA} h^-(t)\mathrm{d}t \ .$$

□

5.5 Little Multiplier Theorem

We now turn to the proof of the second part of Theorem 5.8. We assume (48) and $\gamma(\mp\infty) = \pm\infty$. The function $\gamma^\star$ and the family $\mathcal{B}M(\gamma)$ were defined in Sect. 5.3. Note that $\gamma^\star$ is decreasing and $\gamma^\star - \gamma \geq 0$.

Lemma 5.10. *If the family $\mathcal{B}M(\gamma)$ is short, then $\gamma^\star - \gamma \in L^1_\Pi$.*

Proof.

$$\int_l \frac{\gamma^\star - \gamma}{1+x^2}\mathrm{d}x \lesssim \frac{1}{\delta(l)^2} \int_0^{|l|} t\mathrm{d}t \asymp \frac{|l|^2}{\delta(l)^2} \ .$$

□

The proof of the little multiplier is extremely simple if we settle for a slightly weaker statement:

$$\sum_{\mathcal{B}M(\gamma)} \frac{|l|^2 \log^+ |l|}{\delta(l)^2} < \infty \quad \Rightarrow \quad N^+[U] \neq 0 \ .$$

Indeed, the last computation shows that in this case we have

$$\int (\gamma^\star - \gamma) \log^+(\gamma^\star - \gamma) \ \mathrm{d}\Pi < \infty \ ,$$

which is a (necessary and) sufficient condition for $(\gamma^\star - \gamma)\tilde{} \in L^1_\Pi$, see [42]. We have a representation

$$\gamma = \gamma^\star + (\gamma - \gamma^\star) ,$$

where the first term is decreasing and the second one is in $\tilde{L}^1_\Pi$, so $N^+[U] \neq 0$ by the basic criterion.

Lemma 5.11 (Main Lemma). *If the family $BM(\gamma)$ is short, then for any given $\epsilon > 0$ there is a function β such that $\beta' \leq \epsilon$ near $\pm\infty$ and*

$$\gamma^\star - \gamma + \beta \in \tilde{L}^1_\Pi .$$

The little multiplier theorem now follows immediately:

$$\gamma(x) - \epsilon x = (\gamma - \gamma^\star - \beta) + (\beta - \epsilon x) + \gamma^\star .$$

The first term is in $\tilde{L}^1_\Pi$, and the last two terms are decreasing at infinities.

Proof (Main Lemma). Denote $f = \gamma^\star - \gamma$, so f is a non-negative function in L^1_Π, $f' \leq$ const, and the family $\mathcal{L} = \mathcal{B}M(\gamma)$ of the components of $\{f \neq 0\}$ satisfies

$$\sum_{l \in \mathcal{L}} \frac{|l|^2}{\delta(l)^2} < \infty .$$

These are the only properties of f that will be used. We will also need the following notation: for an interval $l = [a, b]$ we define its "tent" function

$$T_l(x) = \begin{cases} x - a & a \leq x \leq (a+b)/2 , \\ b - x & (a+b)/2 \leq x \leq b , \\ 0 & x \in \mathbb{R} \setminus l . \end{cases}$$

Note that

$$\|T_l\|_\Pi \gtrsim \frac{|l|^2}{(\delta(l) + |l|)^2} . \tag{55}$$

We will construct disjoint intervals l_n such that $\{f \neq 0\} \subset \bigcup l_n$,

$$\sum_n \frac{|l_n|^2}{\delta(l_n)^2} < \infty , \tag{56}$$

and

$$\forall n \quad \exists \epsilon_n \in [0, \epsilon] , \qquad \int_{l_n} (f - \epsilon_n T_{l_n}) \, \mathrm{d}\Pi = 0 . \tag{57}$$

Let us show that the existence of such intervals l_n implies the main lemma. We will use the easier part of the atomic decomposition technique of Hardy spaces, see [11].

We define

$$\beta = -\sum_n \epsilon_n T_{l_n} , \qquad g = f + \beta ,$$

so β is in $\mathrm{Lip}(\epsilon)$, and all we need to check is that $\tilde g \in L^1_\Pi$ or, in other words, that g belongs to the *real* Hardy space $\mathcal{H}^1_\Pi(\mathbb{R})$. We can represent g as follows:

$$g = \sum \chi_n g = \sum \lambda_n \frac{\chi_n g}{\lambda_n} := \sum \lambda_n A_n \ ,$$

where χ_n is the characteristic function of l_n, and we choose

$$\lambda_n = \Pi(l_n)\ \|\chi_n g\|_\infty \ .$$

It is clear that the functions $A_n = \lambda_n^{-1}(\chi_n g)$ are "atoms":

$$\int A_n \mathrm{d}\Pi = \frac{1}{\lambda_n}\int_{l_n} g\mathrm{d}\Pi = 0 \ ,$$

by (57) and

$$\|A_n\|_\infty = \frac{\|\chi_n g\|_\infty}{\lambda_n} = \frac{1}{\Pi(l_n)} \ .$$

By (56) we also have

$$\sum \lambda_n \lesssim \sum \Pi(l_n)|l_n| \asymp \sum \frac{|l_n|^2}{\delta(l_n)^2} < \infty \ .$$

It follows that $\sum \lambda_n A_n \in \mathcal{H}^1_\Pi(\mathbb{R})$, see [11].

To finish the proof it remains to describe the construction of the intervals $\tilde l_n$ and the slopes ϵ_n. We consider the case where all intervals $l \in \mathcal{L}$ are in $(1,+\infty)$. The construction for intervals in $[-\infty,-1)$ is similar.

Suppose the left endpoint $a_n = a$ of l_n has been constructed, and a is also the left endpoint of some interval $l = (a, b(l)) \in \mathcal{L}$. (To start the induction we take the leftmost endpoint for a_1.) Consider the function

$$F(b) \equiv F_\epsilon(b) = \int_a^b \left[f - \epsilon T_{(a,b)}\right] \mathrm{d}\Pi \ ,$$

and define

$$b_n = \min\{b \geq b(l) :\ f(b) = 0,\ F(b) \leq 0\} \ .$$

For example, if we already have $F(b(l)) \leq 0$, then $b_n = b(l)$. Since $f \in L^1_\Pi$, we have $F(+\infty) = -\infty$ and so $b_n < \infty$. We also define ϵ_n from the equation

$$\int_{a_n}^{b_n} \left[f - \epsilon_n T_{(a_n,b_n)}\right] \mathrm{d}\Pi = 0 \ .$$

Finally, we define a_{n+1} as the leftmost endpoint of all intervals $l \in \mathcal{L}$ to the right of l_n.

It is clear from the construction that the intervals l_n cover $\{f \neq 0\}$, that all ϵ_n's are $\leq \epsilon$, and that we have (57). Let us check (56). We consider three types of intervals l_n:

(a) $F(b_n) < 0$ but $\exists l \in \mathcal{L}$ such that $l \subset l_n$ and $|l|/\delta(l) \asymp |l_n|/\delta(l_n)$,
(b) $F(b_n) = 0$,
(c) other intervals.

Property (56) is obvious for the group (a). For the group (b), we use (55):

$$\sum_{(b)} \frac{|l_n|^2}{(\delta(l_n) + |l_n|)^2} \lesssim \frac{1}{\epsilon} \int_{\cup_{(a)} l_n} f \mathrm{d}\Pi < \infty \, .$$

The argument for the group (c) is similar as long as we can show that the slopes are $> \epsilon/2$, i.e. $F_{\epsilon/2}(b_n) > 0$. Since $F(b_n) < 0$, b_n is by construction the right endpoint of some interval $l \in \mathcal{L}$, and since $l_n \notin (a)$ we have $|l| \ll |l_n|$. Let c be the left endpoint of the above l; by construction, $F(c) > 0$. We have

$$\begin{aligned} F_{\epsilon/2}(b_n) &= \left(\int_{a_n}^{c} + \int_{c}^{b_n} \right) \left[f - \frac{\epsilon}{2} T_{(a,b)} \right] \mathrm{d}\Pi > \int_{a_n}^{c} \left[f - \epsilon T_{(a,c)} \right] \mathrm{d}\Pi \\ &= F(c) > 0 \, . \end{aligned}$$

□

Beurling–Malliavin Density

5.6 Radius of Completeness

Let $\Lambda \subset \mathbb{R}$ and let $\mathcal{E}_\Lambda$ denote the family of exponential functions $\{\mathrm{e}^{\mathrm{i}\lambda t} : \lambda \in \Lambda\}$. By definition, the *radius of completeness* of the family $\mathcal{E}_\Lambda$ is the number

$$R(\Lambda) = \sup \left\{ a : \ \mathcal{E}_\Lambda \text{ is complete in } L^2(0,a) \right\} \, .$$

In terms of Toeplitz kernels, by Proposition 4.4 we have

$$R(\Lambda) = \sup \left\{ a : \ N[\bar{S}^a J_\Lambda] = 0 \right\} \, ,$$

where J_Λ denotes some/any meromorphic inner function J such that $\{J = 1\} = \Lambda$. By the Beurling–Malliavin multiplier theorem we also have

$$R(\Lambda) = \sup \left\{ a : \ N^+[\bar{S}^a J_\Lambda] = 0 \right\} \, .$$

The combination of the second Beurling–Malliavin and the little multiplier theorems, see Theorem 5.8, then gives the following metric characterization of $R(\Lambda)$. By definition, the *Beurling–Malliavin density* of Λ is the number

$$d_{\mathrm{BM}}(\Lambda) = \inf\{a : \gamma_a(\pm\infty) = \mp\infty \text{ and } \mathcal{B}M[\gamma_a] \text{ is short}\} \, ,$$

where $\gamma_a := 2\pi n_\Lambda - at$.

Corollary 5.12. *$R(\Lambda) = d_{\mathrm{BM}}(\Lambda)$.*

5.7 General Transition Parameter Problems

Let M be a unimodular function with non-decreasing continuous argument; we call it a *gap function*. For a given unimodular function $U = \mathrm{e}^{\mathrm{i}\gamma}$ we want to compute the critical exponent

$$\sup\left\{a:\ N[\bar{M}^a U] = 0\right\}\ .$$

This number of course can be $\pm\infty$. The Beurling–Malliavin density theorem corresponds to the case $M = S$ and $U = J$ (or $\bar{S}^c J$). More generally, Theorems 5.4 and 5.8 allow us to compute the transition parameter in the case $M = S$ and $U = \bar{\Theta} J$ where $|\Theta'| \le \text{const}$.

Of course, one can state similar problems concerning families of Toeplitz kernels in other functional spaces. Theorem 5.1 states that the critical exponent is the same in all $\mathcal{H}^p$–spaces if both M and Θ are tempered and the "gap" is wide enough: $N^\infty[b^N \bar{M}^\epsilon] \ne 0$ for all $\epsilon > 0$ and $\forall N$.

One could try to generalize the Beurling–Malliavin theory ($M = S$) to arbitrary gap functions. As a first step it is natural to consider the "*standard*" gap functions $S^{(\alpha)}$ and $S_+^{(\alpha)}$, $\alpha > 0$, defined as follows:

$$S^{(\alpha)}(x) = \begin{cases} S(x^\alpha) & x > 0\ , \\ S(-|x|^\alpha) & x < 0\ , \end{cases} \qquad S_+^{(\alpha)}(x) = \begin{cases} S(x^\alpha) & x > 0\ , \\ S(0) & x < 0\ . \end{cases}$$

Note that these functions satisfy identities like

$$S^{(\alpha)}(kx) = \left[S^{(\alpha)}(x)\right]^{k^\alpha}\ , \qquad (k > 0)\ .$$

For each standard gap function, one would expect to have some kind of a *Beurling–Malliavin theory*, i.e. a combination of theorems that allow to express the transition parameter in terms of the Beurling–Malliavin intervals under an appropriate growth restriction on γ.

Here is a typical example of a transition parameter problem with a standard gap function.

Example 5.13. Let $\mathrm{Ai}(x)$ denote the usual Airy function: it is a solution of the equation $y'' = xy$, which is L^2 at $+\infty$. It is well-known that the Airy function is entire and also

$$\mathrm{Ai}(x) = \sqrt{x} F\left(\frac{2}{3}\mathrm{i}x^{3/2}\right)\ ,$$

for some solution F of the Bessel equation of order $1/3$. If $x = -\lambda$ and $\lambda > 0$, then we have

$$\mathrm{Ai}(-\lambda) = \mathrm{i}\sqrt{\lambda} F\left(\frac{2}{3}\lambda^{3/2}\right) \sim \lambda^{-1/4}\cos\left(\frac{2}{3}\lambda^{3/2} + \text{const}\right)\ , \qquad \lambda \to +\infty\ . \tag{58}$$

Given $\Lambda \subset \mathbb{R}$ we ask if the family of shifts

$$\mathcal{E}_\Lambda = \{\mathrm{Ai}(t-\lambda) : \ \lambda \in \Lambda\}$$

is complete in $L^2(\mathbb{R}_+)$. Note that $u_\lambda(t) = \mathrm{Ai}(t-\lambda)$ is an L^2–solution of the Schrödinger equation

$$-\ddot{u} + tu = \lambda u \ , \qquad t \in \mathbb{R}_+ \ ,$$

so we can apply our general approach, see Sect. 4.1.

Claim. Up to a finite dimensional gap, the family $\mathcal{E}_\Lambda$ is complete in $L^2(\mathbb{R}_+)$ iff

$$N[\bar{M}J_\Lambda] = 0 \ , \qquad M = \left[S_+^{(3/2)}\right]^{2/3} .$$

Proof. According to Sect. 4.1 and Theorem 5.1, the criterion for completeness (up to a finite dimensional gap) is $N[\bar{\Theta}J_\Lambda] = 0$, where Θ is the Weyl inner function. We can replace Θ by M because of the asymptotic formula (58) for $u_\lambda(0) = \mathrm{Ai}(-\lambda)$ and a similar formula for $\dot{u}_\lambda(0)$. □

Remark 5.14. This completeness problem, which involves shifts of a given function in $L^2(\mathbb{R}_+)$) is different from the well-known Wiener problem concerning shifts in $L^2(\mathbb{R})$. The latter is essentially the problem concerning exponential families in weighted L^2–spaces; it can also be restated in terms of Toeplitz kernels.

Let us now state the transition parameter problem. Given Λ, denote by $\mathcal{E}_\Lambda^{(a)}$ the family $\{u_\lambda : \lambda \in \Lambda\}$ of L^2–solutions of the Schrödinger equation with potential $q(t) = t/a$, $(a > 0)$. We want to compute the "radius of completeness" $R(\Lambda)$, i.e. the critical value of a such that $\mathcal{E}_\Lambda^{(a)}$ is complete in $L^2(\mathbb{R}_+)$. In terms of Toeplitz kernels we have

$$R(\Lambda) = \sup\left\{a : \ N[\bar{M}^a J_\Lambda] = 0\right\} \ , \qquad M = \left[S_+^{(3/2)}\right]^{2/3} \ .$$

This is similar to the Beurling–Malliavin situation, which can be reformulated as the completeness problem for the solutions of the Schrödinger equation with $q \equiv 0$ on $[0, a]$:

$$R(\Lambda) = \sup\left\{a : \ N[\bar{M}^a J_\Lambda] = 0\right\} \ , \qquad M = S_+^{(1/2)} \ .$$

In the Airy situation, the parameter a characterizes the "size" of the singularity, which plays the same role as the length of the interval in the regular case.

Transition parameter problems arise also in connection with the spectral theory problems that we discussed in Sect. 4.

Example 5.15. Let L be a regular Schrödinger operator on $[0, 1]$ and let $\Lambda \subset \sigma(L)$. We want to characterize the numbers c such that

(i) the potential on $[0,c]$ and the partial spectrum Λ determine L,
(ii) the potential on $[0,c]$ and the spectral measure on Λ determine L,

see Sect. 4.8. According to the results of Sect. 4.9 (and Theorem 5.1), these questions are equivalent to the transition parameter problems with $M = S_+^{(1/2)}$ – to find the values of

$$\inf\left\{c:\ N\left[\bar{M}^{2(1-c)}J_\Lambda\right]=0\right\}\ ,\qquad \inf\left\{c:\ N\left[\bar{M}^{2(1-c)}J_\Lambda^2\right]=0\right\}\ ,$$

in the cases (i) and (ii) respectively.

Indeed, in the case (i), Λ has to be defining for Φ, the Weyl function corresponding to the restriction of the potential to $[c,1]$, which means that $N[\bar{\Phi}^2 J_\Lambda]=0$ within the admissible gap. Also, we can replace Φ by $M^{(1-c)}$. In the case (ii), we use the same argument for the divisor $2\chi_\Lambda$.

5.8 Square Root Transformation

The following construction and its corollaries in this and the next subsections are meant to give some idea of what the Beurling–Malliavin theories of standard gap functions may look like.

Let $U = \mathrm{e}^{\mathrm{i}\gamma}$ be a unimodular function such that $\gamma = 0$ on $\mathbb{R}_-$, and let $U_* = \mathrm{e}^{\mathrm{i}\gamma_*}$ be a unimodular function with an *odd* argument related to γ by the equation

$$\gamma_*(t) = \gamma(t^2)\ ,\qquad (t \ge 0)\ .$$

Proposition 5.16. $N^\infty[U] \ne 0 \quad \Leftrightarrow \quad N^\infty[U_*] \ne 0.$

Proof. $\Leftarrow$ Suppose we have $U_* H = \bar{G}$ on $\mathbb{R}$ for some $H, G \in \mathcal{H}^\infty$. Then we also have $U_* H^\flat = \bar{G}^\flat$, where we use the notation

$$H^\flat(z) = \overline{H(-\bar{z})}\ .$$

(Note $U_* = U_*^\flat$.) Thus we have

$$U_* F = \bar{F}^\flat\ ,\qquad F := H + G^\flat\ .$$

Consider now the functions $f, g \in H^\infty(\mathbb{C}_+)$,

$$f(z) = F(\sqrt{z})\ ,\qquad g(z) = \bar{F}(\sqrt{\bar{z}})\ ,$$

where the square root denotes the conformal map $\mathbb{C}\setminus\mathbb{R}_+ \to \mathbb{C}_+$. Let us check that $Uf = \bar{g}$ on $\mathbb{R}$. If $t > 0$, then $f(-t^2) = F(\mathrm{i}t)$ and $g(-t^2) = \bar{F}(\mathrm{i}t)$, so

$$\frac{\bar{g}(-t^2)}{f(-t^2)} = 1 = U(-t^2)\ .$$

On the other hand, $f(t^2) = F(t)$ and $g(t^2) = \bar{F}(-t) = F^\flat(t)$, and therefore

$$\frac{\bar{g}(t^2)}{f(t^2)} = \frac{\bar{F}^\flat(t)}{F(t)} = U_*(t) = U(t^2) \ .$$

$\Rightarrow$ Suppose $Uf = \bar{g}$ on $\mathbb{R}$ for some $f, g \in H^\infty$. Since $U \equiv 1$ on $\mathbb{R}_-$, the analytic functions $f \in H^\infty(\mathbb{C}_+)$ and $g^\# \in H^\infty(\mathbb{C}_-)$ match on $\mathbb{R}_+$ and therefore define a function in $\mathbb{C}\backslash\mathbb{R}_+$. Applying the square root transformation, we get $F \in H^\infty(\mathbb{C}_+)$,

$$F(z) = \begin{cases} f(z^2) & \Re\, z > 0 \ , \\ g^\#(z^2) & \Re\, z < 0 \ . \end{cases}$$

Let us check that $U_*F = \bar{F}^\flat$ on $\mathbb{R}$. If $x > 0$, then $F(x) = f(x^2)$, $\bar{F}^\flat(x) = F(-x) = \bar{g}(x^2)$ and

$$\frac{\bar{F}^\flat(x)}{F(x)} = \frac{\bar{g}(x^2)}{f(x^2)} = U(x^2) = U_*(x) \ .$$

On the other hand, if $x < 0$, then $F(x) = \bar{g}(x^2)$, $\bar{F}^\flat(x) = F(-x) = f(x^2)$ and

$$\frac{\bar{F}^\flat(x)}{F(x)} = \frac{f(x^2)}{\bar{g}(x^2)} = \frac{1}{U(x^2)} = U_*(x) \ .$$

$\square$

The square root transformation makes it possible to derive the Beurling–Malliavin theory of the gap function $M = S_+^{(1/2)}$ from Theorems 5.4 and 5.8 (we also use Theorem 5.1).

Corollary 5.17. *Let $U = \mathrm{e}^{\mathrm{i}\gamma} = \bar{\Theta}J$ and suppose that both Θ and J have bounded arguments at $-\infty$. Suppose in addition*

$$(\arg \Theta)'(t) \le \frac{\text{const}}{\sqrt{t}} \ , \qquad t \to +\infty \ .$$

(i) If $\gamma(t) \not\to -\infty$ as $t \to +\infty$, or if $\gamma(+\infty) = -\infty$ but the family $\mathcal{B}M(\gamma)$ is long, then

$$\forall \epsilon > 0 \ , \qquad N\left[\left(S_+^{(1/2)}\right)^\epsilon U\right] = 0 \ .$$

(ii) If $\gamma(+\infty) = -\infty$ and the family $\mathcal{B}M(\gamma)$ is short, then

$$\forall \epsilon > 0 \ , \qquad N\left[\left(\bar{S}_+^{(1/2)}\right)^\epsilon U\right] \neq 0 \ .$$

Here we consider only the Beurling–Malliavin intervals in $\mathbb{R}_+$, and the meaning of the terms “long” and “short” is the same as in Sect. 5.3.

Example 5.18. Let L be the Schrödinger operator on $\mathbb{R}$ with potential $q(t) = t^2/4$ ("quantum harmonic oscillator") and let $\Lambda \subset \sigma(L) = \mathbb{N} - \frac{1}{2}$. We want to find the critical value c_* of real numbers c such that q on $(-\infty, -c)$ and the spectral measure on Λ (including the numbering of eigenvalues) determine L, see Sect. 4.8. We can explicitly compute c_* in terms of Beurling–Malliavin intervals if the set Λ satisfies the inequality

$$\#(\Lambda \cap l) \geq \frac{|l|}{2} - \text{const} , \qquad (59)$$

for all intervals $l = [a, b] \subset \mathbb{R}_+$ such that $b \leq a + \sqrt{a}$.

Claim.

$$c_* = \inf\{c : \gamma_c(+\infty) = -\infty \text{ and } \mathcal{B}M[\gamma_c] \text{ is short}\} ,$$

where $\gamma_c := 2n_\Lambda(t) - t - 2c\sqrt{t}$.

Sketch of Proof: Let Θ be the Weyl inner function corresponding to the restriction of the potential to $\mathbb{R}_+$, so Θ^2 is essentially the same (i.e. up to a finite dimensional gap) as S_+. Then the Weyl inner function corresponding to $(-c, \infty)$ is essentially the same as $\Phi = \Theta M^c$, where $M = S_+^{(1/2)}$. The data determine L if the divisor $2\chi_\Lambda$ is defining for $K[\Phi^2]$, i.e. (again up to a finite dimensional gap)

$$N[\bar{M}^{2c}U] = 0 , \qquad U = \bar{S}_+ J_\Lambda^2 .$$

Note that

$$\gamma(t) \equiv \arg U(t) = 2n_\Lambda(t) - t + O(1) , \qquad (t > 0) .$$

To apply the corollary, we need to make sure that $\gamma(t)$ does not drop by more than a constant on each interval l described in the statement. This is exactly our condition (59).

Let us state another corollary, which gives a necessary condition for the non-triviality of a Toeplitz kernel in the "one-sided" situation.

Corollary 5.19. *Let $U = \mathrm{e}^{\mathrm{i}\gamma}$ and $\gamma = 0$ on $\mathbb{R}_-$. If $N^\infty[U] \neq 0$, then*

$$\int_{\{\gamma > A\}} \frac{\mathrm{d}t}{t\sqrt{t}} = \frac{o(1)}{A} , \qquad A \to +\infty , \qquad (60)$$

in particular

$$\gamma^+ \in L^p\left(\frac{\mathrm{d}t}{1 + t\sqrt{t}}\right) , \qquad (0 < p < 1) .$$

Proof. Consider the square root transform U_*. By the basic criterion, $N^+[U_*] \neq 0$ implies

$$\Pi\{\gamma_* > A\} = \frac{o(1)}{A} , \qquad A \to +\infty .$$

□

One can state similar results for tempered γ's satisfying $\gamma = O(1)$ at $-\infty$: if $N^p[U] \neq 0$, then we have (60) at $+\infty$.

5.9 Final Thoughts

Except for the "two-sided" case $M = S$ and the "one-sided" case $M = S_+^{(1/2)}$, the complete Beurling–Malliavin theory of the standard gap functions is not known. Here we mention some preliminary considerations.

Two facts seem to be certain. First, the theories should be different in the subexponential case ($\alpha < 1$ for two-sided gap functions and $\alpha < 1/2$ for one-sided functions) and superexponential case ($\alpha > 1$ and $\alpha > 1/2$ respectively). Second, the role of the Smirnov class $\mathcal{N}^+$ in the case $S^{(\alpha)}$, $\alpha \neq 1$, is not the same as in the classical case $M = S$. One should probably introduce appropriate "Smirnov classes" for all $\alpha < 1$, e.g. the preimage of $\mathcal{N}^+$ under the square root transformation in the case $\alpha = 1/2$, cf. the last corollary.

Case 5.20 (Subexponential case). We have the following partial results. From the last corollary we immediately derive

Corollary 5.21. *Let* $M = S^{(1/2)}$ *and* $U = \mathrm{e}^{\mathrm{i}\gamma}$*. Suppose*

$$\gamma'(x) \geq -\frac{C}{\sqrt{|x|}}\,, \qquad x \to \pm\infty\,.$$

If $\gamma(\mp\infty) = \pm\infty$ *and the family* $\mathcal{B}M(\gamma)$ *is short, then*

$$\forall \epsilon > 0\,, \qquad N^\infty\left[\bar{M}^\epsilon U\right] \neq 0\,.$$

Applying the square root transformation one more time we get

Corollary 5.22. *Let* $M = S^{(1/4)}$ *and* $U = \mathrm{e}^{\mathrm{i}\gamma}$*. Suppose*

$$\gamma'(x) \geq -C|x|^{-3/4}\,, \qquad x \to \pm\infty\,.$$

If $\gamma(\mp\infty) = \pm\infty$ *and the family* $\mathcal{B}M(\gamma)$ *is short, then*

$$\forall \epsilon > 0\,, \qquad N^\infty\left[\bar{M}^\epsilon U\right] \neq 0\,.$$

These facts should extend to all $S^{(\alpha)}$ with $\alpha < 1$. The "converse" statements (if true) should follow from Theorem 5.9 in appropriate "Smirnov classes".

Case 5.23 (Superexponential case). We only discuss the gap function S_+, which corresponds to the two-sided case $M = S^{(2)}$. The proof of Thorem 5.8 applies verbatim to give the following criterion in the class $\mathcal{N}^+$.

Proposition 5.24. *Let* $U = \mathrm{e}^{\mathrm{i}\gamma}$*. Suppose* γ *is bounded on* $\mathbb{R}_-$ *and* $\gamma' \geq -\mathrm{const}$ *on* $\mathbb{R}_+$*.*

(i) If $\gamma \not\to -\infty$ *at* $+\infty$*, or if* $\gamma(+\infty) = -\infty$ *but* $\mathcal{B}M(\gamma)$ *is long, then*

$$\forall \epsilon > 0\,, \qquad N^+\left[S_+^\epsilon U\right] = 0\,.$$

(ii) If $\gamma(+\infty) = -\infty$ and $\mathcal{B}M(\gamma)$ is short, then

$$\forall \epsilon > 0 , \qquad N^{+}\left[\bar{S}_{+}^{\epsilon} U\right] \neq 0 .$$

On the other hand, it is *false* that we have $N^{\infty}\left[\bar{S}_{+}^{\epsilon} U\right] \neq 0$ in the case (ii). (Of course, we still have $N^{\infty}\left[u\bar{S}^{\epsilon}\right] \neq 0$.) The criterion in $\mathcal{H}^{\infty}$ should involve a different definition of long families, probably the following:

$$\sum_{l \in \mathcal{B}M(\gamma)} \frac{|l|^2}{\delta(l)^{3/2}} = \infty . \tag{61}$$

Let us state a partial result in the language of $S^{(2)}$. Note that under the square root transformation, the condition (61) becomes

$$\sum_{l \in \mathcal{B}M(\gamma)} \frac{|l|^2}{\delta(l)} = \infty .$$

We get the exactly this condition if we apply the non-rigorous argument preceding the proof of Theorem 5.9.

Proposition 5.25. *Let $M = S^{(2)}$ and $U = \mathrm{e}^{\mathrm{i}\gamma}$. Suppose*

$$\gamma'(x) \geq -C|x| , \qquad x \to \pm\infty .$$

(i) If $\gamma(x) \not\to \pm\infty$ as $x \to \mp\infty$, or if $\gamma(\mp\infty) = \pm\infty$ but

$$\sum_{l \in \mathcal{B}M(\gamma)} \frac{|l|^2}{\delta(l)(1 + \log^{+}|l|)} = \infty ,$$

then

$$\forall \epsilon > 0 , \qquad N^{+}\left[M^{\epsilon} U\right] = 0 .$$

(ii) If $\gamma(+\infty) = -\infty$ and

$$\sum_{\mathcal{B}M(\gamma)} \frac{|l|^2 \log^{+}|l|}{\delta(l)} < \infty ,$$

then

$$\forall \epsilon > 0 , \qquad N^{+}\left[\bar{M}^{\epsilon} U\right] \neq 0 .$$

Example 5.26. Let L be the harmonic oscillator considered in Example 5.18, and let $\Lambda \subset \sigma(L)$. The first part of the last proposition provides a sufficient condition for the fact that q on $\mathbb{R}_{-}$ and the spectral measure on Λ determine L. This condition is less precise than the one stated in Example 5.18 because we have a larger gap, which characterizes the singularity at infinity rather than the extra length of the known part of the spectrum. On the other hand, the condition in the above proposition does not require any extra assumptions on Λ, cf. (59).

In conclusion, we mention that the study of gap functions which are less regular than the standard ones (or even arbitrary) is an interesting and probably difficult problem.

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Heat Measures and Unitarizing Measures for Berezinian Representations on the Space of Univalent Functions in the Unit Disk

Paul Malliavin

10 rue Saint Louis en l'Isle, 75004 Paris, France sli@ccr.jussieu.fr

1 Introduction

From the sixties Lennart Carleson is for me the undisputed leader of Analysis of my generation; he helped me personally in many occasions; I feel very honored to have been called to participate to his seventy fifth Birthday Conference which, by the quality of the talks, have been for me a memorable event; I express all these personal feelings by dedicating this paper to Lennart together with the article [3].

The Lebesgue measure on $\mathbb{R}^d$ can be characterized by its invariance under translation; from this invariance is built the algebraic properties of the Fourier transform and subsequently the whole theory of Euclidean Harmonic Analysis.

Harmonic Analysis of finite dimensional Lie group is based on the existence of a left invariant measure: the Haar measure. It has been proved by André Weil [16] that *any measurable group having a σ–additive left invariant measure is, as measurable space, isomorphic to a locally compact group equipped with its classical Haar measure.*

Our purpose is to investigate *quasi-invariance in the context of a given representation* as a substitute to the concept of *invariance* in order to try to construct an integration theory fitting infinite dimensional Lie algebras coming from mathematical physics. The paper concludes with a section called "Perspectives" in the spirit of this Conference where Lennart invited everybody of us to look towards new adventures.

2 Gaussian Representation of Heisenberg Commutation Relations

We present in this first section some well known facts. As a commutation relation we will use the Heisenberg relation $[p, q] = h$, where h denotes the Planck constant. To this commutation relation is associated the 3–dimensional

Lie algebra generated by the three elements, p, q, c with the commutation relations

$$[p, q] = ch\ , \qquad [p, c] = 0\ , \qquad [q, c] = 0\ ,$$

the corresponding group being the 3–dimensional Heisenberg group, group which we will not write down in this paper essentially concerned with Lie algebra.

By a rescaling of the variables (p, q), we can reduce ourself to the case $h = 1$: the remaining of this section will be written taking $h = 1$.

We consider on $\mathbb{R}$ the algebra of $\mathcal{D}$ the C^∞ functions with compact support. We define a representation ρ of the Heisenberg algebra on $\mathcal{D}$ by defining

$$\rho(p)(\phi)(x) := \phi'(x)\ , \qquad \rho(q)(\phi)(x) := x\phi(x) - \phi'(x)\ , \qquad \rho(c)\phi = \phi\ .$$

Then ρ is a Lie algebra homomorphism

$$\rho(p)\rho(q) - \rho(q)\rho(p) = \rho(c)\ .$$

A *unitarizing measure of the representation* ρ is defined as the data of a probability measure μ on R such that, denoting the adjoint of the operator a on L^2_μ by a^* we have

$$(\rho(p))^* = \rho(q)\ .$$

Proposition 2.1. *The unitarizing measure of* ρ *exists, is unique and is equal to the Gaussian measure*

$$\gamma(\mathrm{d}x) = \frac{1}{\sqrt{2\pi}} \exp\left(-x^2/2\right) \mathrm{d}x\ .$$

Proof. By integration by parts we obtain

$$(\phi' \mid \psi) = \int_R \phi'\psi\gamma(\mathrm{d}x) = \int_R [-\phi\psi' + x\phi\psi]\gamma(\mathrm{d}x)\ .$$

This identity shows that the Gaussian measure is unitarizing.

Uniqueness. Consider the elliptic operator

$$\mathcal{L} := -\rho(q)\rho(p)\ .$$

Then

$$(\mathcal{L}\phi)(x) = \phi''(x) - x\phi'(x)\ ,$$

and $\mathcal{L}$ satisfies the basic intertwining relation

$$\mathrm{d} \circ \mathcal{L} = -\mathrm{d} + \mathcal{L} \circ \mathrm{d}\ .$$

Exponentiating this relation by the heat semi-group $\exp(t\mathcal{L})$, we find that for any $\phi \in \mathcal{D}$

$$\mathrm{d}\left(\exp(t\mathcal{L})\phi\right) = \exp(-t) \times \exp(t\mathcal{L})\phi'\ .$$

Therefore denoting by $\pi_t(x_0, \mathrm{d}x)$ the fundamental solution of the heat operator we get that

$$\lim_{t\to+\infty} \int \pi_t(x_0, \mathrm{d}x)\phi(x)$$

exists and is independent of x_0.

For any unitarizing measure μ we must have

$$\lim_{t\to+\infty} \int \pi_t(x_0, \mathrm{d}x)\phi(x) = \int \phi(x)\mu(\mathrm{d}x) ,$$

a relation which proves the uniqueness.

It is clear that the uniqueness proof given above furnishes also existence.

□

The $(2d+1)$–dimensional Lie algebra having as basis c the central element and p_k, q_k, $k \in [1, d]$, satisfying $[p_k, q_s] = \delta_k^s c$, where δ_k^s denotes the Kronecker symbol has a unitary representation on $L^2_{\gamma_d}(\mathbb{R}^d)$ where $\gamma_d = \gamma\otimes\cdots\otimes\gamma$ is the d–dimensional Gaussian measure. This representation is obtained by making the product of the previously obtained representation of the Heisenberg algebra.

2.1 Infinite Dimensional Heisenberg Commutation Relations

Consider the ∞–dimensional Lie algebra having as basis c the central element and p_k, q_k, $k = 1, \ldots$, satisfying $[p_k, q_s] = \delta_k^s c$, where δ_k^s denotes the Kronecker symbol. Consider the infinite dimensional Gaussian measure γ_∞, i.e. the probability on the probability space X generated by an infinite sequence of independent scalar Gaussian variables.

Let us associate to a constant vector field z the translation by $\tau_\epsilon : x \mapsto x + \epsilon z$. The vector z is said to be *admissible* if the measure γ_∞ is z *quasi-invariant*, which means that $(\tau_\epsilon)_*\gamma_\infty$ is absolutely continuous relatively to γ_∞ for all ϵ. Denote

$$l^2 = \{z;\ \|z\|_{l^2} = \sum [z_k]^2 < \infty\} .$$

Theorem 2.2 (Cameron–Martin). *The set of admissible vectors is equal to l^2. For $z \in l^2$ the series $(z \mid x) = \sum_k z_k x_k$ converges γ_∞ almost everywhere and*

$$(\tau_\epsilon)_*\gamma_\infty = [1 + \epsilon(z \mid x) + o(\epsilon)]\gamma_\infty , \qquad \text{as } \epsilon \to 0 .$$

Remark 2.3. A fundamental difference with the finite dimensional case is that the vector space l^2 of γ_∞–admissible vector fields satisfies $\gamma_\infty(l^2) = 0$.

Theorem 2.4 (Integration by Parts). *For every smooth function ϕ*

$$\int_X (D_z\phi)(x)\gamma(\mathrm{d}x) = \int_X \phi(x)(z \mid x)\gamma(\mathrm{d}x) .$$

Remark 2.5. As in the 1–dimensional case, it is possible to construct an elliptic operator in infinite dimension which is symmetric in L^2_ν for each measure satisfying the formula of integration by parts

$$\int_X (D_z\phi)(x)\nu(\mathrm{d}x) = \int_X \phi(x)(z\,|\,x)\nu(\mathrm{d}x) \ .$$

Then it is possible to deduce that the set of such measures ν contains only one element: the Gaussian measure γ_∞.

Theorem 2.6. *The Gaussian measure in infinite dimension can be characterized by the associated formula of integration by parts.*

Remark 2.7. This statement is parallel to the characterization of the Haar measure by its invariance by translation.

Mathematical Physics provides a beautiful algebraic structure: the Virasoro algebra, together with natural holomorphic representations; these algebraic structure can be considered as the "skeleton". The challenge is to realize some *"flesh around a skeleton"* that is to construct a *measured space* on which the algebraic action can naturally be realized. Our point of view will be to solve the following

Inverse Problem. Construct (and characterize) a probability measure μ through the a priori data $\delta_\mu(Z)$.

Here $Z \in \mathcal{Z}$ is a sufficiently large family of a priori given vector fields and $\delta_\mu(Z)$ is the *divergence of Z relatively to μ*, which is defined by the following formula of integration by parts

$$\int \langle Z, \mathrm{d}\phi\rangle \mathrm{d}\mu = \int \delta_\mu(Z)\phi \mathrm{d}\mu \ .$$

In the case of an a priori given representation, $\mathcal{Z}$ will be the Lie algebra of the infinitesimal action and $\delta_\mu(Z)$ the automorphy factor of the action.

3 Quantization Above Symplectic Groups

3.1 The Lowest Dimensional Case: The Poincaré Disk

Consider the unit disk of the complex plane D. The Poincaré metric together with its complex structure generates the canonical symplectic form

$$\omega = (1-|z|^2)^{-2}\mathrm{d}z \wedge \mathrm{d}\bar{z} \ ,$$

for which D has a structure of a Kähler manifold. The Kähler potential is

$$K(z) = -\log(1-|z|^2) \ ,$$

which satisfies $\partial\bar{\partial}K = \omega$.

Denote by $\mathrm{SU}(1,1)$ the group of complex matrices

$$\begin{pmatrix} a & b \\ \bar{b} & \bar{a} \end{pmatrix} ,$$

such that $|a|^2 - |b|^2 = 1$. This group acts on D by

$$z \mapsto \frac{az+b}{\bar{b}z+\bar{a}} .$$

The symplectic form ω is invariant under this group action. The isotropy group of the point $0 \in D$ is the rotation group; the symplectic form ω is invariant under rotations; therefore identifying the tangent space at 0 to D with the quotient of $\mathfrak{su}(1,1)$ the Lie algebra of $\mathrm{SU}(1,1)$, by the rotation group, we can lift ω to a canonic bilinear form $\tilde{\omega}$ defined on $\mathfrak{su}(1,1)$.

Denote by $\mathrm{d}v = (1-|z|^2)^{-2}\mathrm{d}z \wedge \mathrm{d}\bar{z}$ the Riemannian volume of the Poincaré disk and consider the one parameter family of volume measures

$$\mathrm{d}\rho_h = \exp(-hK)\mathrm{d}v ,$$

where h will be called the Planck constant. Then $\rho_h(1) < \infty$ for $h > 1$ and then, by rescaling, it can be looked upon as a probability measure. The measure ρ_h is not invariant under the infinitesimal action of $\mathfrak{su}(1,1)$. Under this action appears the modulus of quasi-invariance given by h times the derivative of K.

Denote $\mathcal{H}L^2_{\rho_h}$ the space of holomorphic functions on D which are square integrable for the measure ρ_h. The holomorphic connection ∇ is defined by

$$\nabla_h = \frac{\partial}{\partial z} - h\bar{\partial}K .$$

The Lie algebra $\mathfrak{su}(1,1)$ acts unitarily on $\mathcal{H}L^2(L;\rho_h)$ through ∇_h. This action provides a representation of the Lie algebra $\widetilde{\mathfrak{su}}(1,1)$, the central extension of $\mathfrak{su}(1,1)$, which is the Lie algebra of dimension 4 obtained by adding to $\mathfrak{su}(1,1)$ a central element c and where the bracket is defined by

$$[\eta_1,\eta_2]^* = [\eta_1,\eta_2] + c \times h\tilde{\omega}(\eta_1,\eta_2) .$$

Within this paradigm the Heisenberg algebra appears as the central extension of the abelian two dimensional Lie algebra.

This paradigm has been developed by Berezin [5] in the context of Siegel theory of automorphic functions; this finite dimensional theory is the stepping stone for the infinite dimensional theory sketched in the next section.

3.2 Sato Infinite Dimensional Symplectic Geometry

Let V denote the vector space of real valued C^1–functions defined on the circle S^1 with zero mean value. Define

$$\omega(u,v) = \frac{1}{\pi}\int_0^{2\pi} uv'\mathrm{d}\theta\ , \qquad u,v \in V\ .$$

On V the Hilbert transform $\mathcal{J}$: $\sin(k\theta) \mapsto \cos(k\theta)$, $\cos(k\theta) \mapsto -\sin(k\theta)$, defines a complex structure and an Hilbertian metric

$$\|u\|^2 := -\omega(u, \mathcal{J}u)\ .$$

Then

$$\left\|\sum_k a_k \cos(k\theta) + b_k \sin(k\theta)\right\|^2 = \sum_k k(a_k^2 + b_k^2)\ .$$

Let $H = V \otimes \mathbb{C}$ and let H^+ be the eigenspace of the orthogonal transformation $\mathcal{J}$ associated to the eigenvalue $\sqrt{-1}$. Then $H^+ \simeq$ functions having an holomorphic extension inside the unit disk. The bilinear form ω extends to $\tilde{\omega}$ defined on H; it defines a symmetric $\mathbb{C}$–bilinear form on $H \times H$ by

$$\langle h_1, h_2\rangle = (h_1 \,|\, \bar{h}_2)\ , \quad \text{then } (h_1 \,|\, h_2) = \langle h_1, \bar{h}_2\rangle\ ,$$
$$\tilde{\omega}(h_1, h_2) = \langle h_1^+, h_2^-\rangle - \langle h_1^-, h_2^+\rangle\ .$$

3.3 The Group Sp(∞)

Any automorphism U of V extends to an endomorphism $\tilde{U}$ of H. Denoting π^+, π^- the projection of H on H^+, H^- let us introduce

$$a := \pi^+\tilde{U}_g\pi^+\ , \qquad b := \pi^+\tilde{U}_g\pi^-\ .$$

Note that $\tilde{U}$ commutes with the conjugation

$$\tilde{U} = \begin{pmatrix} a & b \\ \bar{b} & \bar{a} \end{pmatrix}\ .$$

The conservation of the symplectic form $\tilde{\omega}$ is equivalent to the relations

$$a^T\bar{a} - b^\dagger b = \pi^+\ , \qquad a^T\bar{b} - b^\dagger a = 0\ ,$$

$a^\dagger$, a^T denoting respectively the adjoint and the transpose of a.

We call the collection of bounded operators $a \in \mathrm{End}(H^+)$, $b \in \mathcal{L}_2(H^-;H^+)$ satisfying these relations the *symplectic group of infinite order* and denote it by $\mathrm{Sp}(\infty)$.

3.4 Infinite Dimensional Siegel Disk

Let

$$\mathcal{D}_\infty := \{Z \in \mathcal{L}((H^-, H^+);\ Z^T = Z,\ 1 - \bar{Z}Z > 0\}\ ,$$

with the condition $\mathrm{trace}(\bar{Z}Z) < \infty$ and define a mapping $\mathcal{D}(\infty) \mapsto \mathrm{End}(H)$ by

$$Z \mapsto \begin{pmatrix} 0 & Z \\ 0 & 0 \end{pmatrix}\ .$$

Theorem 3.1. Sp(∞) *operates on* $\mathcal{D}_\infty$ *by*

$$Z \mapsto Y = (aZ + b)(\bar{b}Z + \bar{a})^{-1} .$$

The orbit through Sp(∞) of the matrix $Z_0 = 0$ is the space of matrices of the form

$$\{b(\bar{a}^{-1})\} = \mathcal{D}(\infty) .$$

3.5 Kähler Potentials

The Kähler potential on $\mathcal{D}_\infty$ is

$$K(Z) := -\log\det(1 - \bar{Z}Z) = -\operatorname{trace}\log(1 - \bar{Z}Z) .$$

The Kähler potential K is lifted to Sp(∞) by

$$\tilde{K}\left[\begin{pmatrix} a & b \\ \bar{b} & \bar{a} \end{pmatrix}\right] = \operatorname{trace}\log(1 + (b)^\dagger b) .$$

The complex Hessian $\partial\bar{\partial}K$ is invariant under the Sp(∞) action. At the origin of $\mathcal{D}(\infty)$ this complex Hessian coincides with the symplectic form $\tilde{\omega}$. Denote the Lie algebra of Sp(∞) by $\mathfrak{sp}(\infty)$.

The *Berezinian representation of* $\mathfrak{sp}(\infty)$, is defined as the infinitesimal action on holomorphic functions on $\mathcal{D}(\infty)$ through the holomorphic connection $\nabla_h = \partial - h \times \bar{\partial}K$.

The problem of *unitarizing measure* is to find a probability μ for which this Berezinian representation is unitary in $\mathcal{H}L^2_\mu$.

The complex Hessian $\partial\bar{\partial}K$ defines an invariant Riemann–Kähler metric on $\mathcal{D}(\infty)$. For this Riemannian metric *the Ricci tensor is identically equal to* $-\infty$, a fact which implies the non existence of a Brownian motion on $\mathcal{D}(\infty)$[*], and which consequently rules out the possibility of constructing unitarizing measure for the Berezinian representations.

We shall resume in the next section the quest for unitarizing measure by restricting Berezinian representations to some subgroup of Sp(∞).

4 Symplectic Geometry on the Group of Diffeomorphisms of the Circle

Denote the unit circle by S^1 and consider the infinite dimensional group

$$\mathrm{Diff}(S^1) := \{\text{orientation preserving diffeomorphisms of } S^1\} .$$

The diffeomorphism group has an action on V the space of functions with vanishing mean value on S^1 defined by

$$U_{g^{-1}}(u) = g^*u - \frac{1}{2\pi}\int_0^{2\pi} (g^*u)\mathrm{d}\theta ,$$

where $(g^*u)(\theta) := u(g(\theta))$.

Theorem 4.1 ([12]). *The map* $g \mapsto U_g$ *defines a homomorphism of* $\mathrm{Diff}(S^1)$ *into* $\mathrm{Sp}(\infty)$.

Proof. This follows from the elementary identity $\omega(U_g(u), U_g(v)) = \omega(u, v)$. □

Let us define the Kähler potential

$$\hat{K}(g) := \tilde{K}(U_g) = \log\det(1 + b_g^\dagger b_g) ,$$

where b_g is the operator associated to the infinite matrix

$$c_{j,k}(g) = \frac{1}{2\pi}\int_0^{2\pi} \exp\left(-\sqrt{-1}(j\theta + kg^{-1}(\theta))\right) \mathrm{d}\theta , \qquad j,k > 0 .$$

4.1 Lie Algebra $\mathfrak{diff}(S^1)$ of $\mathrm{Diff}(S^1)$

We observe that the vector fields $\phi(\theta)\frac{\mathrm{d}}{\mathrm{d}\theta}$ satisfy the identities

$$[\phi_1, \phi_2] = \phi_1\dot{\phi}_2 - \phi_2\dot{\phi}_1 ,$$
$$[\mathrm{e}^{\mathrm{i}n\theta}, \mathrm{e}^{\mathrm{i}m\theta}] = \mathrm{i}(m-n)\mathrm{e}^{\mathrm{i}(n+m)\theta} .$$

Theorem 4.2. *The function* $\hat{K}$ *defines a semi-definite left invariant metric on* $\mathrm{Diff}(S^1)$*, essentially equivalent to the* $H^{3/2}$ *Sobolev-norm.*

Proof. $(\partial_v c_{j,k})(\mathrm{e}) = 0$ if v is a vector of type $(0,1)$; then

$$\langle(\partial\bar{\partial}K)(\mathrm{e}), \mathrm{e}^{\mathrm{i}n\theta} \wedge \mathrm{e}^{-\mathrm{i}n\theta}\rangle = \sum_{k,l} \frac{l}{k} k^2 \mathbb{1}_{(k+l=n)}$$
$$= \sum_{k+l=n} kl = \frac{1}{6}(n^3 - n) .$$

□

5 Canonical Brownian Motion on the Diffeomorphism Group of the Circle

Let us define a sequence of maps $e_n : \mathbb{R}^2 \to \mathfrak{diff}(S^1)$

$$e_n(\xi) = \sqrt{\frac{6}{n^3 - n}}(\xi^1 \cos n\theta + \xi^2 \sin n\theta) , \qquad n > 1 .$$

Let X_k be independent copies of Wiener space of the $\mathbb{R}^2$–valued Brownian motion; define $X = \bigotimes X_k$ and consider the Stratanovitch SDE

$$\mathrm{d}g_x(t) = \left(\sum_k e_k \mathrm{d}x_k(t)\right) \circ g_x(t) , \qquad g_x(0) = I .$$

5.1 Abel Regularization

The Able Regularization of the SDE is

$$\mathrm{d}g_x^r(t) = \left(\sum_k r^k e_k(\mathrm{d}x_k(t))\right) \circ g_x^r(t) \ , \qquad g_x^r(0) = I \ .$$

From Kunita theory it is clear that $g_x^r(t) \in \mathrm{Diff}(S^1)$, $\forall r < 1$.

Theorem 5.1 (Existence of the Brownian Motion). *Denoting $\mathcal{H}(S^1)$ the group of homeomorphisms of S^1, then*

$$\lim_{r\to 1} g_x^r(t) := \gamma_{x,t} \in \mathcal{H}(S^1) \ ,$$
$$\gamma_{x,t}(\theta) - \gamma_{x,t}(\theta') = O(|\theta - \theta'|^{\exp(-t)}) \ ,$$

and the laws ρ_t of $\gamma_x(t)$ satisfy $\rho_t * \rho_{t'} = \rho_{t+t'}$.

Proof. See [13], [4] and [8]. □

The Beurling–Ahlfors [6] quasi-symmetry condition

$$\sup_{t,t'} \left| \frac{\Psi(t+t') - \Psi(t)}{\Psi(t) - \Psi(t-t')} \right| < \infty \ ,$$

is ruled out by the following Theorem.

Theorem 5.2. *Almost surely*

$$\limsup_{h\to 0} \frac{1}{\sqrt{\log^- |h|}} \left(\sup_{t\in[0,1],\, \theta\in S^1} \log \left| \frac{\gamma_{x,t}(\theta+h) - \gamma_{x,t}(\theta)}{\gamma_{x,t}(\theta) - \gamma_{x,t}(\theta-h)} \right| \right) = \log 2 \ .$$

The expression of $\hat{K}$ is not very convenient for the explicit computation of the holomorphic connection $\bar{\partial}\hat{K}$; it is therefore difficult to explicitly compute the restriction of the Berezinian connection ∇_h to $\mathrm{Diff}(S^1)$. This difficulty will be overcome in the next paragraph in the context of the univalent function model.

6 The Manifold of Univalent Functions

We denote by $\mathcal{F}$ the vector space of functions f which are holomorphic in the unit disk $D := \{z; |z| < 1\}$ and C^∞ on its closure $\bar{D}$ and such that $f(0) = 0$; we denote by $\mathcal{F}_0$ the subspace of functions of f satisfying $f'(0) = 0$. We denote

$$\mathcal{U} := \{f \in \mathcal{F};\ f'(0) = 1 \text{ and } f \text{ injective on } \bar{D}\} \ .$$

The representation

$$f(z) = z\left(1 + \sum_{n=1}^{+\infty} c_n z^n\right)$$

introduces the affine coordinates $f \mapsto \{c_*\}$.

Theorem 6.1. *There exists an identification of* $\mathcal{U}$ *with* $\mathrm{Diff}(S^1)/S^1$.

Proof (by C^∞–conformal sewing). Given $f \in \mathcal{U}$, we denote $\Gamma = f(\partial D)$. Then Γ is a smooth Jordan curve which splits the complex plane into two connected open sets: Γ^+ which contains 0 and Γ^- which contains the point at infinity. By the Riemann mapping theorem there exists an holomorphic map $\phi_f : D^c \to \bar{\Gamma}^-$ such that $\phi_f(\infty) = \infty$, ϕ being holomorphic nearby ∞.

A diffeomorphism $g_f \in \mathrm{Diff}(S^1)$ is defined by

$$g_f(\theta) := (f^{-1} \circ \phi_f)(\mathrm{e}^{\mathrm{i}\theta}) .$$

□

Theorem 6.2 (Kirillov [11]). *The Lie algebra* $\mathfrak{diff}(S^1)$ *acts on* $\mathcal{U}$ *by*

$$\mathcal{K}_v(f)(z) := \frac{f^2(z)}{2\pi} \int_{\partial D} \left[\frac{tf'(t)}{f(t)}\right]^2 \frac{v(t)}{f(t) - f(z)} \frac{\mathrm{d}t}{t} .$$

Denote by ∂_k the holomorphic partial derivative relative to the the affine coordinate c_k. Then, for $k > 0$,

$$\mathcal{K}_{\exp(\mathrm{i}k\theta)} := L_k = \partial_k + \bar{\partial}_k + \sum_{n=1}^{+\infty} (n+1)(c_n \partial_{k+n} + \bar{c}_n \bar{\partial}_{k+n}) .$$

6.1 A Differential Form on Diff(S^1)

Associate to $v \in \mathfrak{diff}(S^1)$ the right invariant tangent vector field to $\mathrm{Diff}(S^1)$, $(v^l)_g := \exp(\epsilon v) g$; define the 1–differential form

$$\langle v^l, \Omega \rangle_g = \frac{1}{\pi} \int_{\partial D} S_f(t) v(\log t) t^2 \frac{\mathrm{d}t}{t} ,$$

where S_f is the Schwarzian derivative:

$$S_f := \frac{f'''}{f'} - \frac{3}{2} \left(\frac{f''}{f'}\right)^2 =: \sum_{n \geq 0} z^n P_{n+2}(c_1, \ldots, c_{n+2}) ,$$

where the P_* are polynomials, which satisfy the Neretin [14] recursion formula

$$L_k P_n = (n+k) P_{n-k} + \frac{k^3 - k}{12} \delta_k^n , \qquad P_0 = P_1 = 0 .$$

Theorem 6.3 ([2]).

$$\Omega_g = \bar{\partial} \left(\log \det(I + b^\dagger(g^{-1}) b(g^{-1}))\right) = \bar{\partial} \hat{K} .$$

Theorem 6.4 ([14]). *Denote by ρ_h the Berezinian representation associated to the value h of the Planck constant; then ρ_h can be realized as the projective representation of $\mathfrak{Diff}(S^1)$ on the vector space $\mathcal{H}(\mathcal{U})$ of holomorphic functionals on $\mathcal{U}$ defined by*

$$\rho_h\left(\mathrm{e}^{ik\theta}\right)\Phi = \sqrt{-1}L_k\Phi \;,$$
$$\rho_h\left(\mathrm{e}^{-ik\theta}\right) = \sqrt{-1}(L_{-k} + hP_k)\Phi \;,$$

for all $k > 0$.

Theorem 6.5 ([2]). *A probability measure μ is unitarizing for ρ_h if and only if the corresponding divergences are given by*

$$\delta_\mu(\mathcal{K}_{\cos k\theta})(f) = h\Im P_k \;, \qquad \delta_\mu(\mathcal{K}_{\sin k\theta}) = h\Re P_k \;.$$

6.2 A Process for which the Unitarizing Measure will be Invariant

Define $y = \sum_{k>1} \epsilon_k x_k$, where

$$\epsilon_{2k} = \frac{1}{\sqrt{k^3 - k}} \cos k\theta \;, \qquad \epsilon_{2k+1} = \frac{1}{\sqrt{k^3 - k}} \sin(k\theta) \;,$$

and where x_k is an infinite sequence of independent scalar valued Brownian motions.

The *unitarizing SDE* will be defined as the SDE

$$\mathrm{d}g_y(t) = (\circ\, \mathrm{d}y - hZ\mathrm{d}t)g_y^\rho(t) \;,$$
$$Z = \frac{1}{2}\sum_{k>1}\langle \epsilon_k, \Omega\rangle \partial^l_{\epsilon_k} \;.$$

Theorem 6.6. *The vector Z satisfies $\sup_\theta |Z(\theta)| \leq 24$ and there exists a constant C such that*

$$|Z(\theta) - Z(\theta + \eta)| < C\eta \log\frac{1}{\eta} \;.$$

Remark 6.7. These bounds are obtained using standard techniques of the theory of univalent functions; on the other hand it seems very hard to obtain them by differentiating determinants.

These bounds on Z do not give information how Z depends upon g_y and therefore not sufficient for proving the existence of solutions to the unitarizing SDE.

6.3 When Heat Measure Converges Towards Invariant Measure

Theorem 6.8 ([7]). *Let M be a finite dimensional Riemannian Manifold, Δ its Laplacian, Z a vector field and*

$$\mathcal{L}f = \frac{1}{2}(\Delta f - (Z \,|\, \mathrm{d}f)) \,.$$

Assume that there exists an $\epsilon > 0$ such that

$$\mathrm{Ricci}_M + \nabla Z + (\nabla Z)^* > \epsilon \times \mathrm{Identity} \,.$$

When $t \to \infty$ the heat measure $\pi_t(m_0, \mathrm{d}m)$ converges towards an invariant measure μ satisfying $\int \mathcal{L}f \mathrm{d}\mu = 0$. Assume that Z is a gradient vector field. Then

$$\int_M D_Y f \mathrm{d}\mu = \int_M f((Z \,|\, Y) - \nabla_* Y^*)\mathrm{d}\mu \,.$$

Theorem 6.9 (Bowick–Rajeev). *Ricci of* $\mathrm{Diff}(S^1)$ *exists and is equal to the negative identity.*

The real Hessian of the Kähler potential $\hat{K}$ has three components $(2,0)$, $(1,1)$, $(0,2)$ the third being the conjugate of the first. The fact that $\hat{K}$ is the Kähler potential means that the Hessian of type $(1,1)$ is equal to the identity. Therefore from the Theorem of Bowick–Rajeev we get positivity for the $(1,1)$ component when the value of the Planck constant is greater than 1. *Unfortunately it is not possible to complete this argument because it does not care about the* $(2,0)$ *component of the Hessian.* Conceptually, an existence theorem for invariant measures where the hypothesis of real convexity is replaced by a hypothesis of holomorphic convexity is presently lacking.

7 Canonical Brownian Motion on the Manifold of Univalent Functions

We have shown that the canonical Brownian motion "on" $\mathrm{Diff}(S^1)$, $\gamma_{x,t}$, takes its values in the group of homeomorphisms of S^1; therefore we cannot apply the theory of C^∞ conformal sewing. More generally conformal sewing is possible when the quasi-symmetry condition of Beurling–Ahlfors is satisfied; but almost surely $\gamma_{x,t}$ never satisfy this condition. The main objective of this section is to realize a conformal sewing for $\gamma_{x,t}$. We shall adapt the strategy used for C^∞–sewing to the stochastic case, taking advantage of the fact that the time appearing in the stochastic flows furnishes a natural deformation parameter, in the spirit of the Loewner equation. This deformation will linearize infinitesimally the underlying the Beltrami equations and this linearized equation will be solved by the Cauchy integral formula.

7.1 Beurling–Ahlfors Extension of a Vector Field on the Circle to the Disk

Consider the kernel B defined on $\mathbb{R}$ by the formula $B(2s) = \sin^2 s/s^2$ and denote by B' its derivative. Consider the complex valued Brownian motion

$$X_n(t) := \begin{cases} \frac{1}{2}(x_{2n}(t) - \mathrm{i}x_{2n+1}(t)) \ , & n > 0 \ , \\ \bar{X}_n(t) \ , & n < 0 \ . \end{cases}$$

Consider the random vector field define on the unit disk D by the formula

$$Z_{x,t}(z) = \mathrm{i}z \sum_{|n|\neq 0,1} \frac{1}{\sqrt{|n|(n^2-1)}} \left[B(n \log \frac{1}{|z|}) + 6B'(n \log \frac{1}{|z|}) \right] \mathrm{e}^{\mathrm{i}n\theta} X_n(t) \ ,$$

where $\theta = \Im \log z$.

Theorem 7.1 ([3]). *The restriction of $Z_{x,t}$ to $|z| = 1$ coincides with the random vector field defining the canonical Brownian motion "on"* $\mathrm{Diff}(S^1)$. *The random vector field $Z_{x,t}$ generates a stochastic flow of homeomorphisms of D, denoted by $\Psi_{x,t}$ which preserves the circle where it coincides with $\gamma_{x,t}$.*

There exist numerical strictly positive constants c_1, c_2 such that

$$E \left[d_t(\bar{\partial} Z_{x,t})(z) * d_t(\bar{\partial} Z_{x,t})(z') \right] \leq c_1 \exp(-c_2 d(z,z')) \ ,$$

where $d(z,z')$ is the Poincaré hyperbolic distance on D.

7.2 Stochastic Beltrami Equation

Recall that the factor of pseudo conformality of a diffeomorphism u is defined as $\Theta_u := \frac{\bar{\partial} u}{\partial u}$.

Theorem 7.2 ([3]). *There exists a diffeomorphism $F_{x,t}$ of $\mathbb{C}$ such that*

$$\Theta_{F_{x,t}}(z) = \begin{cases} \Theta_{\Psi_{x,t}}(z) \ , & z \in D \ , \\ 0 \ , & z \notin D \ . \end{cases}$$

Proof (Outline). By composition formula for quasi-conformal modulus we have $f_{x,t} := F_{x,t} \circ \Psi_{x,t}^{-1}$ is holomorphic in D

$$\bar{\partial}[F_{x,t} \circ \Psi_{x,t}^{-1}] = 0 \ .$$

We use the time as a deformation parameter, denoting by δ_t the Stratonovitch differentials. Following Lowner introduce $U_t = \delta_t(F_{x,t}) \circ F_{x,t}^{-1}$. As the left multiplicative differential of the flow $\Psi_{x,t}$ is $Z_{x,t}$ we get

$$\bar{\partial} U_t = \alpha \bar{\partial} Z_{x,t} \circ f_{x,t}^{-1} =: A_{x,t} \ , \qquad |\alpha| = 1 \ .$$

As the support of U_t is compact, we get the following expression for U_t

$$U_t(\zeta) = \frac{1}{2\mathrm{i}\pi} \int_{F_{x,t}(D)} \frac{1}{\zeta - \zeta'} A_{x,t}(\zeta')\mathrm{d}\zeta' \wedge \mathrm{d}\bar{\zeta}' .$$

The conservation of the hyperbolic distance by a conformal map leads to

$$|E(A_{x,t}(\zeta_1)A_{x,t}(\zeta_2))| \le c_1 \exp(-c_2 d(\zeta_1, \zeta_2)) ,$$

an estimate which makes possible to integrate the non Markovian stochastic flow generated by U_t and gives the existence of $F_{x,t}$ and of $f_{x,t} := F_{x,t} \circ \Psi_{x,t}$.

Conclusion. The map $t \mapsto f_{x,t}$ defines a stochastic process with values in $\mathcal{U}$: the canonical Brownian motion on the space of univalent functions. □

8 Perspectives

We shall present in this section prospects of future developments.

8.1 Stochastic Differential Equations with Low Regularity

The classical framework for local existence and uniqueness of an SDE is done under the assumption of a local Lipschitz condition. The construction of the Brownian motion "on" the diffeomorphism group of the circle has stimulated a new theory, [9], [15], valid for SDE on $\mathbb{R}^d$

$$\mathrm{d}\xi_x^k(t) = \sigma_i^k(\xi_x(t))\mathrm{d}x^i(t) + c^k(\xi_x(t))\mathrm{d}t ,$$

where the coefficients satisfy the following regularity conditions

$$\|\sigma(\xi) - \sigma(\eta)\| \le c\|\xi - \eta\| \times \sqrt{|\log\|\xi - \eta\||} ,$$
$$\|c(\xi) - c(\eta)\| \le c\|\xi - \eta\| \times |\log\|\xi - \eta\|| .$$

8.2 The Generalized Bieberbach Problem

Let $\mathcal{U}$ denote the set of normalized univalent functions. We define a map $\psi_n : \mathcal{U} \to \mathbb{C}^n$ by associating to $f \in \mathcal{U}$ its n first nontrivial Taylor coefficients. Denote $\mathcal{A}_n$ the range of ψ_n. We want to characterize effectively $\mathcal{A}_n$. For the first values of n this problem has been solved by Schiffer–Spencer. By De Branges Theorem $\mathcal{A}_n$ is bounded. The space $\mathcal{U}$ is connected: if $f \in \mathcal{U}$ then $f_a(z) = f(az)$ belongs to $\mathcal{U}$ for all $a < 1$.

The elliptic operator driving the Brownian motion on $\mathcal{U}$ has as second order symbol

$$\Delta := \sum_{k>1} \frac{1}{k^3 - k} \; L_{-k}L_k .$$

Denote π_t the law at time t of the Brownian motion on $\mathcal{U}$ starting from the identity at time 0 and denote $(\psi_n)_*\pi_t = \pi_t^n$. The support of π_t^n is contained in $\bar{\mathcal{A}}_n$ and *it seems likely that this inclusion is an equality.* H. Airault has shown that π_t^n is the fundamental solution of a non autonomous heat operator associated to the non autonomous elliptic operator whose symbol Δ_t^n is obtained by taking the conditional expectation for the measure π_t^n of Δ. As the support of μ_n is compact the symbol Δ_t^n must degenerate at the boundary of this support. Therefore *it seems likely that the boundary of $\mathcal{A}_n$ is contained in the set where the real dimension of the space generated $\Re L_k^c$, $\Im L_k^c$, $k \in [1, n]$ is smaller that $2n$.* As generating functions for the L_k have been constructed, this procedure could give computable expressions in finite terms of the boundary of $\mathcal{A}_n$ for all n.

8.3 Universal Teichmüller Space

Let γ be the subalgebra of $\mathfrak{diff}(S^1)$ generated by $\cos\theta, \sin\theta$. Then the corresponding group is the group $\Gamma \simeq \mathrm{SU}(1,1)$ of Möbius transformations.

The *universal Teichmüller space* is defined [10], [1] as

$$\mathcal{T} = \Gamma \setminus \mathrm{Diff}(S^1)/S^1 \; .$$

Theorem 8.1. *$\mathcal{T}$ is isomorphic to the space of Jordan curves having a conformal radius relatively to the origin equal to* 1*. Furthermore there exists on $\mathcal{T}$ a canonical Riemannian metric.*

The existence of heat measure on $\mathcal{T}$ makes possible to define corresponding Sobolev spaces and in some sense a canonical differential calculus on $\mathcal{T}$.

On the other hand is it possible from the Brownian motion on $\mathcal{U}$ to produce a Brownian motion on $\mathcal{T}$?

8.4 Infinite Dimensional Harmonic Analysis

On the Poincaré disk Berezinian representations are linked to automorphic functions; more generally in any finite dimension, Berezinian representations are linked to the Siegel automorphic functions. What could be the infinite dimensional counterpart on $\mathcal{T}$?

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On Local and Global Existence and Uniqueness of Solutions of the 3D Navier–Stokes System on $\mathbb{R}^3$

Ya. G. Sinai

Mathematics Department, Princeton University, USA and Landau Institute of Theoretical Physics, Russian Academy of Sciences `sinai@math.princeton.edu`

To L. Carleson

1 Introduction

Three-dimensional Navier–Stokes system (NSS) on $\mathbb{R}^3$ without external forcing is written for the velocity vector $u(x,t) = (u_1(x,t), u_2(x,t), u_3(x,t))$ satisfying the incompressibility condition $\operatorname{div} u = 0$ and for the pressure $p(x,t)$ and has the form

$$\frac{\mathrm{D}u}{\mathrm{d}t} = \nu\Delta u - \nabla p\ , \qquad x \in \mathbb{R}^3,\ \ t \geqslant 0\ . \tag{1}$$

Here

$$\left(\frac{\mathrm{D}u}{\mathrm{d}t}\right)_i = \frac{\partial u_i}{\partial t} + \sum_{k=1}^{3} \frac{\partial u_i}{\partial x_k} u_k$$

and $\nu > 0$ is the viscosity. In this paper we take $\nu = 1$.

After Fourier transform

$$v(k,t) = \int_{\mathbb{R}^3} \mathrm{e}^{-\mathrm{i}\langle k,x\rangle} u(x,t)\mathrm{d}x\ ,$$

$$u(x,t) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} v(k,t)\mathrm{e}^{\mathrm{i}\langle k,x\rangle}\mathrm{d}k\ ,$$

$v(k,t) \perp k$ for any $k \in \mathbb{R}^3$ in view of incompressibility and NSS takes the form

$$\frac{\partial v(k,t)}{\partial t} = -|k|^2 v(k,t) + \mathrm{i}\int_{\mathbb{R}^3} \langle k, v(k-k',t)\rangle P_k v(k',t)\mathrm{d}k'\ , \tag{2}$$

where P_k is the orthogonal projection to the subspace orthogonal to k. Clearly,

$$\langle k, v(k-k',t)\rangle = \langle k', v(k-k',t)\rangle \, .$$

We can reduce the system (2) to the system of non-linear integral equations

$$\begin{aligned} v(k,t) = \exp(-|k|^2 t)v_0(k) + \mathrm{i}\int_0^t \exp(-|k|^2(t-\tau))\mathrm{d}\tau \\ \times \int_{\mathbb{R}^3} \langle k, v(k-k',\tau)\rangle P_k v(k',\tau)\mathrm{d}k' \, , \end{aligned} \tag{3}$$

where $v_0(k)$ is the initial condition.

Many problems of hydrodynamics assume the power-like behavior of functions v near $k=0$ and infinity. In this connection it is natural to introduce the spaces $\Phi(\alpha,\omega)$ where $v(k) \in \Phi(\alpha,\omega)$ if

1. $v(k) = \dfrac{c(k)}{|k|^\alpha} \qquad \text{for } |k| \leqslant 1, \;\; c(k) \perp k$
   and $c(k)$ is bounded and continuous outside $k=0$; put $c = \sup\limits_{|k|\leqslant 1} |c(k)|$;
2. $v(k) = \dfrac{d(k)}{|k|^\omega} \qquad \text{for } |k| \geqslant 1$
   and $d(k)$ is bounded and continuous, $d = \sup\limits_{k \geqslant 1} |d(k)|$.

Certainly 1 plays no essential role in this definition and can be replaced by any other fixed number. We shall use the metric $\|v\| = c + d$.

In some cases v can have infinite energy or enstrophy. Therefore classical existence or uniqueness results like the theorem by T. Kato (see [3]) cannot be applied to the spaces $\Phi(\alpha,\omega)$.

In this paper we consider $0 \leqslant \alpha < 3$, $\omega \geqslant 2$ and in Sect. 2 we prove the following theorems.

Theorem 1.1. *Let $\omega > 2$. Then for any $v \in \Phi(\alpha,\omega)$ there exists $t_0 = t_0(\alpha,\omega)$ such that the system* (3) *has a unique solution on the interval $0 \leqslant t \leqslant t_0$ with the initial condition v.*

Theorem 1.2. *Let $\omega > 2$ and $t_0 > 0$ be given. There exists $h > 0$ such that for any $\|v\| < h$ there exists a unique solution of* (2) *on the interval $0 \leqslant t \leqslant t_0$ which has v as the initial condition.*

Our methods do not allow to prove the global existence results in the spaces $\Phi(\alpha,\omega)$ if $\|v\|$ is sufficiently small. There are some reasons to believe that the corresponding statement is even wrong (see Sect. 4). Some results in this direction were obtained recently by E.I. Dinaburg and Yu. Bakhtin.

In Sect. 3 we consider the case $\alpha = \omega = 2$. A stronger statement is valid.

Theorem 1.3. *If $\|v\|$ is sufficiently small then there exists the unique solution of* (3) *with this initial condition for all $t \geqslant 0$.*

Theorem 1.3 was proven earlier by Le Jan and Sznitman [4] and Cannone and Planchon [2] (see also the review by M. Canone [1]). Our methods do not allow to prove for $\alpha = \omega = 2$ the existence of local solutions if $\|v\|$ is large. Probably, this statement is also wrong.

In Sect. 4 we consider $v(k) = c(k)/|k|^\alpha$ for $2 < \alpha < 3$, $\omega = \alpha$ and discuss some possibilities for blow-ups in these cases.

During the proofs there appear various constants whose exact values play no role in the arguments. We denote them by capital A with various subindexes.

2 Local Existence and Uniqueness Theorems

We shall prove theorems 1.1 and 1.2 simultaneously pointing out the differences in the arguments at the end of this section. We shall construct solutions of (3) by the method of successive approximations. Put $v^{(0)}(k,t) = \exp(-|k|^2 t)v_0(k)$ and define for $n > 0$

$$\begin{aligned} v^{(n)}(k,t) = v^{(0)}(k,t) + \mathrm{i}\int_0^t \exp(-|k|^2(t-\tau))\mathrm{d}\tau \\ \times \int\limits_{\mathbb{R}^3} \left(k, v^{(n-1)}(k-k',\tau)\right) P_k v^{(n-1)}(k',\tau)\mathrm{d}k' \,. \end{aligned} \tag{4}$$

Clearly, $v^{(n)}(k,t) \perp k$. It follows from (3) that

$$\begin{aligned} v^{(n+1)}(k,t) - v^{(n)}(k,t) = \mathrm{i}\int_0^t \exp(-|k|^2(t-\tau))\mathrm{d}\tau \\ \times \int\limits_{\mathbb{R}^3} \Big[\left(k, v^{(n)}(k-k',t) - v^{(n-1)}(k-k',t)\right) P_k v^{(n)}(k',\tau) \\ + \left(k, v^{(n-1)}(k-k',\tau)\right) P_k \left(v^{(n)}(k',\tau) - v^{(n-1)}(k',\tau)\right)\Big] \mathrm{d}k' \,. \end{aligned} \tag{5}$$

From (4)

$$\begin{aligned} \left|v^{(n)}(k,t)\right| \leqslant \left|v^{(0)}(k,t)\right| + \int_0^t \exp(-|k|^2(t-\tau))\mathrm{d}\tau \\ \times |k| \int\limits_{\mathbb{R}^3} \left|v^{(n-1)}(k-k',\tau)\right| \left|v^{(n-1)}(k',\tau)\right| \mathrm{d}k' \\ = \left|v^{(0)}(k,t)\right| + \frac{1}{|k|} \int\limits_0^{t|k|^2} \mathrm{e}^{-\tau}\mathrm{d}\tau \\ \times \int\limits_{\mathbb{R}^3} \left|v^{(n-1)}\left(k-k', t-\frac{\tau}{|k|^2}\right)\right| \left|v^{(n-1)}\left(k', t-\frac{\tau}{|k|^2}\right)\right| \mathrm{d}k' \,. \end{aligned} \tag{6}$$

We shall prove that if $v^{(n-1)}(k,\tau) \in \Phi(\alpha,\omega)$ and $\left\|v^{(n-1)}(k,\tau)\right\| \leqslant h$ for all $0 \leqslant \tau \leqslant t$ then $v^{(n)}(k,\tau) \in \Phi(\alpha,\omega)$ and we shall derive the estimate for $\left\|v^{(n)}(k,\tau)\right\|$ provided that t is small enough.

We shall write $v_0^{(n-1)}(k,\tau)$ if $|k| \leqslant 1$ or $v_1^{(n-1)}(k,\tau)$ if $|k|>1$ instead of $v^{(n-1)}(k,\tau)$ and assume that $v_0^{(n-1)}(k,\tau)=0$ if $|k|>1$, $\;v_1^{(n-1)}(k,\tau)=0$ if $|k| \leqslant 1$. Consider two cases.

Case 1. $|k| \leqslant 1$. We have from (6)

$$\begin{aligned}
\left|v^{(n)}(k,t)\right| |k|^{\alpha} \leqslant \|v_0\| + |k|^{\alpha-1} \int\limits_0^{t|k|^2} \mathrm{e}^{-\tau}\mathrm{d}\tau \\
\times \Bigg[\int\limits_{\mathbb{R}^3} \left|v_0^{(n-1)}\left(k-k', t-\frac{\tau}{|k|^2}\right)\right| \left|v_0^{(n-1)}\left(k', t-\frac{\tau}{|k|^2}\right)\right| \mathrm{d}k' \\
+ 2\int\limits_{\mathbb{R}^3} \left|v_0^{(n-1)}\left(k-k', t-\frac{\tau}{|k|^2}\right)\right| \left|v_1^{(n-1)}\left(k', t-\frac{\tau}{|k|^2}\right)\right| \mathrm{d}k' \\
+ \int\limits_{\mathbb{R}^3} \left|v_1^{(n-1)}\left(k-k', t-\frac{\tau}{|k|^2}\right)\right| \left|v_1^{(n-1)}\left(k', t-\frac{\tau}{|k|^2}\right)\right| \mathrm{d}k' \Bigg] \\
\leqslant \|v_0\| + |k|^{\alpha-1}\left(1-\exp(-t|k|^2)\right) h^2 \times \Bigg[\int\limits_{\substack{|k'|\leqslant 1 \\ |k-k'|\leqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\alpha}|k'|^{\alpha}} \\
+2 \int\limits_{\substack{|k'|\geqslant 1 \\ |k-k'|\leqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\alpha}|k'|^{\omega}} + \int\limits_{\substack{|k'|\geqslant 1 \\ |k-k'|\geqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\omega}|k'|^{\omega}} \Bigg] \,. \qquad (7)
\end{aligned}$$

Each of these integrals will be estimated separately.

The first integral of (7).

$$\int\limits_{\substack{|k'|\leqslant 1 \\ |k-k'|\leqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\alpha}|k'|^{\alpha}} = |k|^{3-2\alpha} \int\limits_{\substack{|k'|\leqslant 1/|k| \\ \left|k/|k|-k'\right|\leqslant 1/|k|}} \frac{\mathrm{d}k'}{\left|\frac{k}{|k|}-k'\right|^{\alpha}|k'|^{\alpha}} \,.$$

Concerning the last integral we can write

$$\int\limits_{\substack{|k'|\leqslant 1/|k| \\ \left|k/|k|-k'\right|\leqslant 1/|k|}} \frac{\mathrm{d}k'}{\left|\frac{k}{|k|}-k'\right|^{\alpha}|k'|^{\alpha}} \leqslant \begin{cases} A_1(\alpha)\,, & \text{if } \alpha > \frac{3}{2}\,, \\ A_1(\alpha)\ln\frac{1}{|k|}\,, & \text{if } \alpha = \frac{3}{2}\,, \\ A_1(\alpha)|k|^{-3+2\alpha}\,, & \text{if } \alpha < \frac{3}{2}\,. \end{cases}$$

From these inequalities it follows that for $|k| \leqslant 1$, $t \leqslant t_0$

$$|k|^{\alpha-1}\left(1-\exp(-t|k|^2)\right) \int\limits_{\substack{|k'|\leqslant 1\\ |k-k'|\leqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^\alpha |k'|^\alpha}$$

$$\leqslant |k|^{2-\alpha}\left(1-\exp(-t|k|^2)\right) \int\limits_{|k'|\leqslant 1/|k|} \frac{\mathrm{d}k'}{\left|\frac{k}{|k|}-k'\right|^\alpha |k'|^\alpha} \leqslant t_0 A_2(\alpha) \,. \quad (8)$$

The second integral of (7).

$$\int\limits_{\substack{|k'|\geqslant 1\\ |k-k'|\leqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^\alpha |k'|^\omega} = |k|^{3-\alpha-\omega} \int\limits_{\substack{|k'|\geqslant 1/|k|\\ \left|k/|k|-k'\right|\leqslant 1/|k|}} \frac{\mathrm{d}k'}{|k'|^\omega \left|\frac{k}{|k|}-k'\right|^\alpha} \,.$$

It is clear that $|k/|k|-k'| \geqslant |k'|-1$. Therefore in the domain of integration $|k'| \leqslant 1+1/|k|$ and

$$\int \frac{\mathrm{d}k'}{|k'|^\omega \left|\frac{k}{|k|}-k'\right|^\alpha} \leqslant \int\limits_{1/|k|\leqslant |k'|\leqslant 1+1/|k|} \frac{\mathrm{d}k'}{|k'|^\omega \left|\frac{k}{|k|}-k'\right|^\alpha} \leqslant |k|^\omega A_3(\alpha,\omega) \,.$$

Returning back to (7) we can write

$$|k|^{\alpha-1}\left(1-\exp(-t|k|^2)\right) \int\limits_{\substack{|k'|\geqslant 1\\ |k-k'|\leqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^\alpha |k|^\omega} \leqslant t_0 A_4(\alpha,\omega) \,.$$

The third integral of (7). The estimate of this integral is even simpler:

$$\int\limits_{\substack{|k'|>1\\ |k-k'|>1}} \frac{\mathrm{d}k'}{|k'|^\omega |k-k'|^\omega} \leqslant A_5(\omega) \,,$$

since $\omega > 2$. Therefore

$$|k|^{\alpha-1}\left(1-\exp(-t|k|^2)\right) \int\limits_{\substack{|k'|\geqslant 1\\ |k-k'|\geqslant 1}} \frac{\mathrm{d}k'}{|k|^\omega |k-k'|^\omega} \leqslant t A_6(\alpha,\omega) \,.$$

Finally for $|k| \leqslant 1$ we get

$$\left|v^{(n)}(k,t)\right| |k|^\alpha \leqslant \|v_0\| + t_0 h^2 A_7(\alpha,\omega) \,. \quad (9)$$

Case 2. $1 \leqslant |k| \leqslant 1/\sqrt{t_0}$. From (6)

$$\left|v^{(n)}(k,t)\right| |k|^{\omega} \leqslant \|v_0\| + h^2 |k|^{\omega-1}\left(1-\exp(-t|k|^2)\right)$$
$$\times \left[\int\limits_{\substack{|k'|\leqslant 1\\ |k-k'|\leqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\alpha}|k'|^{\alpha}} \right. \tag{10}$$
$$\left. + \int\limits_{\substack{|k'|\geqslant 1\\ |k-k'|\leqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\alpha}|k'|^{\omega}} + \int\limits_{\substack{|k'|\geqslant 1\\ |k-k'|\geqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\omega}|k'|^{\omega}} \right] .$$

The first term in (10) can be non-zero for $1 \leqslant |k| \leqslant 2$ and in this case it is not more than

$$\int\limits_{|k'|\leqslant 1} \frac{\mathrm{d}k'}{|k'|^{\alpha}|k-k'|^{\alpha}} \leqslant A_8(\alpha,\omega) .$$

Therefore in view of $1 \leqslant |k| \leqslant 2$

$$|k|^{\omega-1}\left(1-\exp(-t|k|^2)\right) \int\limits_{\substack{|k'|\leqslant 1\\ |k-k'|\leqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\alpha}|k'|^{\alpha}} \leqslant t_0 A_9(\alpha,\omega) . \tag{11}$$

For the second term in (10) we can write

$$\int\limits_{\substack{|k'|\geqslant 1\\ |k-k'|\leqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\alpha}|k'|^{\omega}} \leqslant \frac{1}{|k|^{\omega}} A_{10}(\alpha,\omega)$$

and this gives

$$|k'|^{\omega-1}\left(1-\exp(-t|k|^2)\right) \int\limits_{\substack{|k'|\geqslant 1\\ |k-k'|\leqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\alpha}|k'|^{\omega}}$$
$$\leqslant |k|^{\omega+1} \times t_0 \times \frac{1}{|k|^{\omega}} A_{11}(\alpha,\omega) = |k| \times t_0 A_{11}(\alpha,\omega) \leqslant \sqrt{t_0} A_{11}(\alpha,\omega) . \tag{12}$$

Consider the last term in (10):

$$\int\limits_{\substack{|k'|\geqslant 1\\ |k-k'|\geqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\omega}|k'|^{\omega}} \leqslant |k|^{3-2\omega} \int\limits_{\substack{|k'|\geqslant 1/|k|\\ k/|k|-k'|\geqslant 1/|k|}} \frac{\mathrm{d}k'}{\left|\frac{k}{|k|}-k'\right|^{\omega}|k'|^{\omega}} . \tag{13}$$

Again this integral is bounded if $\omega < 3$, diverges as $\ln|k|$ if $\omega = 3$ and behaves as $|k|^{\omega-3}$ if $\omega > 3$. Therefore for $\omega < 3$

$$
\begin{aligned}
|k|^{\omega-1}\left(1-\exp(-t_0|k|^2)\right) & \int\limits_{\substack{|k'|\geqslant 1\\ |k-k'|\geqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\omega}|k'|^{\omega}} \\
&\leqslant \text{const} \times |k|^{\omega+1} \times t_0 \times |k|^{3-2\omega} = \text{const} \times |k|^{4-\omega} \times t_0 \\
&\leqslant \text{const} \times t_0^{1-(4-\omega)/2} = \text{const} \times t_0^{(\omega-2)/2} \, .
\end{aligned} \tag{14}
$$

For $\omega = 3$ the last expression is not more than

$$
\text{const} \times t_0 \times |k|^4 \times |k|^{-3} \ln|k| = \text{const} \times t_0 \times |k| \times \ln|k| \leqslant \text{const} \times t_0^{1/3} \, .
$$

In this inequality we could take any power of t_0 less than $1/2$ instead of $1/3$. The value of const depends on this number. Collecting all estimates we can write

$$
\left|v^{(n)}(k,t)\right| |k|^{\omega} \leqslant \|v_0\| + \|h\|^2 t_0^{\delta} A_{12}(\alpha,\omega) \, , \tag{15}
$$

for some positive $\delta > 0$. Remark that here we used the fact that $\omega > 2$.

Case 3. $|k| \geqslant 1/\sqrt{t_0}$. Again from (6)

$$
\begin{aligned}
\left|v^{(n)}(k,t)\right| |k|^{\omega} \leqslant \|v_0\| + h^2 |k|^{\omega-1} \Bigg[& \int\limits_{\substack{|k'|\leqslant 1\\ |k-k'|\leqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\alpha}|k'|^{\alpha}} + \\
& +2 \int\limits_{\substack{|k'|\leqslant 1\\ |k-k'|\geqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\omega}|k'|^{\alpha}} + \int\limits_{\substack{|k'|\geqslant 1\\ |k-k'|\geqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\omega}|k'|^{\omega}} \Bigg] \, .
\end{aligned}
$$

The first integral can be non-zero only if $t_0 > 1$. Therefore it is zero if we discuss theorem 1.1 and consider sufficiently small t_0. If t_0 is not small then h will be small (see below). If $t_0 > 1$ this integral was estimated before (see integral 1 in case 1) and it can be non-zero if $|k| \leqslant 2$. In this case it is bounded and

$$
|k|^{\omega-1} \left[\int\limits_{\substack{|k'|\leqslant 1\\ |k-k'|\leqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\alpha}|k'|^{\alpha}} \right] \leqslant A_{13}(\alpha,\omega) \, .
$$

For the second integral we use the estimate

$$
\int\limits_{\substack{|k'|\leqslant 1\\ |k-k'|\geqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\omega}|k'|^{\alpha}} \leqslant \frac{1}{|k|^{\omega}} A_{14}(\alpha,\omega)
$$

and therefore

$$2|k|^{\omega-1} \int\limits_{\substack{|k'|\leqslant 1\\ |k-k'|\geqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\omega}|k'|^{\alpha}} \leqslant \frac{1}{|k|} A_{15}(\alpha,\omega) \leqslant \sqrt{t_0} A_{15}(\alpha,\omega) \ .$$

For the third integral we can write:

$$\int\limits_{\substack{|k'|\geqslant 1\\ |k-k'|\geqslant 1}} \frac{\mathrm{d}k'}{|k-k'|^{\omega}|k'|^{\omega}} \leqslant \begin{cases} \text{const} \times |k|^{3-2\omega} \ , & \text{if } \omega < 3 \ , \\ \text{const} \times |k|^{-3} \ln |k| \ , & \text{if } \omega = 3 \ , \\ \text{const} \times |k|^{-\omega} \ , & \text{if } \omega > 3 \ . \end{cases}$$

For the first case we also have $|k|^{\omega-1} \times |k|^{3-2\omega} = |k|^{2-\omega} \leqslant t_0^{(\omega-2)/2}$. In all cases

$$|k|^{\omega-1} \int \frac{\mathrm{d}k'}{|k-k'|^{\omega}|k|^{\omega}} \leqslant \frac{\ln |k|}{|k|} A_{16}(\alpha,\omega) \leqslant t_0^{1/3} A_{17}(\alpha,\omega) \ .$$

From all presented estimates it follows that

$$\|v^{(n)}\| \leqslant \|v^{(0)}\| + \|v^{(n-1)}\|^2 t_0^{1/3} A_{17}(\alpha,\omega) \ , \tag{16}$$

where

$$v^{(m)} = \max_{0\leqslant t\leqslant t_0} \|v^{(m)}(k,t)\| \ .$$

Take any $\lambda > 1$, for example, $\lambda = 2$. If $\|v^{(n-1)}\| \leqslant 2\|v_0^{(0)}\|$ then

$$\|v^{(n)}\| \leqslant \|v^{(0)}\| + 4\|v^{(0)}\|^2 t_0^{1/3} A_{17}(\alpha,\omega) = \|v^{(0)}\| \left(1 + 4\|v^{(0)}\| t_0^{1/3} A_{17}(\alpha,\omega)\right)$$

If t_0 is so small that $4\|v^{(0)}\| t_0^{1/3} A_{17}(\alpha,\omega) < 1$ then $\|v^{(n)}\| \leqslant 2\|v_0^{(0)}\|$. On the other hand, if t_0 is given and $\|v^{(0)}\|$ is so small that $\|v^{(0)}\| t_0^{1/3} A_{17}(\alpha,\omega) \leqslant 1$ then $\|v^{(n)}\| \leqslant 2\|v_0^{(0)}\|$. In other words, under conditions of theorems 1.1 and 1.2 all $v^{(n)}(k,t) \in \Phi(\alpha,\omega)$ for all $0 \leqslant t \leqslant t_0$ and $\|v^{(n)}\| \leqslant 2\|v^{(0)}\|$.

Now we shall prove the convergence of all iterations $v^{(n)}$ to a limit as $n \to \infty$ in the sense of our metric.

Consider $|k| \leqslant 1$. We have from (5)

$$\begin{aligned}
&\left|v^{(n+1)}(k,t) - v^{(n)}(k,t)\right| |k|^{\alpha} \\
&\quad \leqslant |k|^{\alpha+1} \int_0^t \exp(-|k|^2(t-\tau))\mathrm{d}\tau \int\limits_{\mathbb{R}^3} \Big[\left|v^{(n)}(k-k',\tau) - v^{(n-1)}(k-k',\tau)\right| \\
&\qquad \times \left(\left|v^{(n)}(k',\tau)\right| + \left|v^{(n-1)}(k-k',\tau)\right|\right) \left|v^{(n)}(k',\tau) - v^{(n-1)}(k',\tau)\right| \Big] \mathrm{d}k' \\
&\quad = |k|^{\alpha+1} \int_0^t \exp(-|k|^2(t-\tau))\mathrm{d}\tau \int\limits_{\mathbb{R}^3} \left(|v^{(n)}(k',\tau)| + |v^{(n-1)}(k',\tau)|\right) \\
&\qquad \times \left|v^{(n)}(k-k',\tau) - v^{(n-1)}(k-k',\tau)\right| \mathrm{d}k' \ .
\end{aligned}$$

We use the estimates of $|v^{(n)}(k',\tau)|$, $|v^{(n-1)}(k',\tau)|$ since $v^{(n-1)}(k',\tau)$, $v^{(n)}(k',t)$ belong to the space $\Phi(\alpha,\omega)$ and $\|v^{(n)}(k',\tau)\|$, $\|v^{(n-1)}(k',\tau)\| \leqslant 2\|v^{(0)}\|$. Denote

$$h^{(n)} = \max_{0\leqslant t\leqslant t_0} \left\| v^{(n)}(k,t) - v^{(n-1)}(k,\tau) \right\| .$$

The same arguments as above show that $h^{(n+1)} \leqslant \varepsilon h^{(n-1)}$ for some $0 < \varepsilon < 1$. Other cases are considered in a similar way. We omit the details. The last inequality gives the convergence of $v^{(n)}$ to the limit. Theorems 1.1 and 1.2 are proven.

3 The Case $\boldsymbol{\alpha = \omega = 2}$

This case is special in several respects. It was considered before by Le Jan and Sznitman [4] and by Cannone and Planchon [2]. The authors proved that if the norm $\|v^{(0)}\|$ is sufficiently small then there exists the unique solution of (2) for all $t \geqslant 0$ having this initial condition.

We shall show how this result can be obtained with the help of technique of Sect. 2. Thus we assume that $v^{(0)}(k) = c(k)/|k|^2$ and denote $c = \sup_{k\in\mathbb{R}^3} |c(k)|$. We shall show that if $c \leqslant c_0$ then the solution of (2) exists for all $t \geqslant 0$, $v(k,t) \in \Phi(2,2)$ and $\|v(k,t)\| \leqslant c_1$ for another constant c_1.

We use the same iteration scheme (4). Take any t_0. Assuming that $v^{(n-1)}(k,t) \in \Phi(2,2)$ for all $0 \leqslant t \leqslant t_0$ we have $v^{(n-1)}(k,t) = c^{(n-1)}(k,t)/|k|^2$, and

$$v^{(n-1)} = \max_{0\leqslant t\leqslant t} \|c^{(n-1)}(k,t)\| .$$

We can write

$$\begin{aligned} &|k|^2|v^{(n)}(k,t)| \\ &\quad \leqslant \|v^{(0)}\| + \|v^{(n-1)}\|^2|k|^3 \int_0^t \exp(-|k|^2(t-\tau))\mathrm{d}\tau \int\limits_{\mathbb{R}^3} \frac{\mathrm{d}k'}{|k-k'|^2|k'|^2} . \end{aligned} \tag{17}$$

It is easy to see that the last integral of (17) is bounded by $A_{18}/|k|$ and substituting this back into the equation we get

$$\begin{aligned} \|v^{(n)}(k,t)\| &\leqslant \|v^{(0)}\| + A_{18}\|v^{(n-1)}\|^2|k|^2 \int_0^t \exp(-|k|^2(t-\tau))\mathrm{d}\tau \\ &= \|v^{(0)}\| + A_{18}\|v^{(n-1)}\|^2 \left(1 - \exp(-|k|^2 t)\right) . \end{aligned}$$

If for some $\lambda > 1$ we have the inequality $\|v^{(n-1)}\| \leqslant \lambda\|v^{(0)}\|$ then

$$\|v^{(n)}(k,t)\| \leqslant \|v^{(0)}\| + \lambda^2 A_{18}\|v^{(0)}\|^2 = \|v^{(0)}\| \left(1 + \lambda^2 A_{18}\|v^{(0)}\|\right).$$

Choose λ so that

$$\left(\lambda - \frac{1}{2A_{18}\|v^{(0)}\|}\right)^2 \leqslant \frac{1}{(2A_{18}\|v^{(0)}\|)^2} - 1 \, ,$$

or

$$\lambda \geqslant \frac{1}{1 - A_{18}\|v^{(0)}\|} \, .$$

Then $\|v^{(n)}\| \leqslant \lambda \|v^{(0)}\|$. In other words, for any such λ all iterations $v^{(n)}(k,t)$ are defined, $v^{(n)}(k,t) \in \Phi(2,2)$ and $\|v^{(n)}(k,t)\| \leqslant \lambda \|v^{(0)}\|$.

Now we have to prove the convergence of $v^{(n)}$ to a limit as $n \to \infty$. Put

$$h^{(n)} = \sup_{0 \leqslant t \leqslant t_0} \sup_{k \in \mathbb{R}^3} \left| v^{(n)}(k,t) - v^{(n-1)}(k,t) \right| |k|^2 \, .$$

We use (5):

$$\begin{aligned} \left| v^{(n+1)}(k,t) - v^{(n)}(k,t) \right| |k|^2 &\leqslant 2\lambda \|v^{(0)}\| \|v^{(n)} - v^{(n-1)}\| |k|^3 \\ &\quad \times \int_0^t \exp(-|k|^2(t-\tau)) \mathrm{d}\tau \int\limits_{\mathbb{R}^3} \frac{\mathrm{d}k'}{|k-k'||k'|^2} \\ &\leqslant 2\lambda A_{18} \|v^{(0)}\| h^{(n)} \end{aligned}$$

Thus if $2\lambda A_{18}\|v^{(0)}\| < 1$ then $h^{(n+1)} \leqslant \lambda A_{18} \|v^{(0)}\| h^{(n)}$ and $h^{(n)}$ tend to zero exponentially fast. This gives the convergence of $v^{(n)}$ to a limit. Remark that we have no restrictions on t_0, i.e. our arguments imply the existence of solutions on any interval of time. C. Fefferman explained to me [1] how in this case the existence of global solutions follows from the existence of local solutions with the help of scaling arguments. It is interesting that presumably for large $|v^{(0)}|$ the local existence theorem may not be valid. Dinaburg and Bakhtin (yet unpublished) showed that if $\|v^{(0)}\|$ is sufficiently small then $v(k,t) \to 0$ as $t \to \infty$ and fixed k.

4 Some Possibilities for Blow-ups in Finite Time in the Spaces $\boldsymbol{\Phi(\alpha,\alpha)}$

We shall consider $v^{(0)}(k) = c^{(0)}(k)/|k|^\alpha$, $k \in \mathbb{R}^3$. It follows from Theorem 1.1 that for sufficiently small t_0 there exists the unique solution of (2) on the interval $[0, t_0]$. Since it is only a local statement there are all reasons to believe that for α close to 3 there can be blow-ups of solutions in finite time. In this section we discuss related possibilities. Take a sequence $\left\{\Delta^{(n)}\right\}$, $\Delta^{(n)} \to 0$ as $n \to \infty$ so that $\sum_n \Delta^{(n)} < \infty$. We shall consider (3) and neglect for small

[1] C. Fefferman, private communication.

values of t by the dependence of $v(k,\tau)$ on τ. In this way we get the sequence of recurrent relations:

$$\begin{aligned} v^{(n+1)}(k) = \exp(-|k|^2\Delta^{(n)})v^{(n)}(k) + \mathrm{i}\int\limits_0^{\Delta^{(n)}} &\exp(-|k|^2(t-\tau))\mathrm{d}\tau \\ &\times \int\limits_{\mathbb{R}^3} \langle k, v^{(n)}(k-k')\rangle P_k v^{(n)}(k')\mathrm{d}k' \ , \end{aligned}$$

or

$$\begin{aligned} c^{(n+1)}(k) = \exp(-|k|^2\Delta^{(n)})c^{(n)}(k) + \mathrm{i}|k|^{\alpha-2}&\left[1-\exp(-|k|^2\Delta^{(n)})\right] \\ &\times \int \frac{\langle k, c^{(n)}(k-k')\rangle P_k c^{(n)}(k')}{|k-k'|^{\alpha}|k'|^{\alpha}}\mathrm{d}k' \ . \end{aligned} \tag{18}$$

The sequence (18) is the main approximation for NSS. We make the following scaling assumptions:

$$c^{(n)}(k) = V^{(n)} f^{(n)}\left(k\sqrt{\Delta^{(n)}}\right) \ ,$$

where $f^{(n)}(\varkappa)$ converge to a limit as $n\to\infty$ and the factor $V^{(n)}$ is chosen so that

$$\sup_{k\in\mathbb{R}^3}\left|f^{(n)}\left(k\sqrt{\Delta^{(n)}}\right)\right| = 1 \ .$$

Then from (18)

$$\begin{aligned} &V^{(n+1)} f^{(n+1)}\left(k\sqrt{\Delta^{(n+1)}}\right) \\ &\quad = \exp(-|k|^2\Delta^{(n)})V^{(n)}f^{(n)}\left(k\sqrt{\Delta^{(n)}}\right) \\ &\quad\quad + \mathrm{i}\left(V^{(n)}\right)^2|k|^{\alpha-2}\left[1-\exp(-|k|^2\Delta^{(n)})\right] \\ &\quad\quad \times \int\limits_{\mathbb{R}^3} \frac{\langle k, f^{(n)}\left((k-k')\sqrt{\Delta^{(n)}}\right)\rangle P_k f^{(n)}\left(k'\sqrt{\Delta^{(n)}}\right)}{|k-k'|^{\alpha}|k'|^{\alpha}}\mathrm{d}k' \ . \end{aligned} \tag{19}$$

Put $\beta^{(n+1)} = V^{(n+1)}/V^{(n)}$ and $\varkappa = k\sqrt{\Delta^{(n)}}$. From (19)

$$\begin{aligned} \beta^{(n+1)} f^{(n+1)}\left(\varkappa\sqrt{\frac{\Delta^{(n+1)}}{\Delta^{(n)}}}\right) &= \exp(-\varkappa^2)f^{(n)}(\varkappa) + \mathrm{i}V^{(n)}\left(\Delta^{(n)}\right)^{(\alpha-2)/2} \\ &\times \left(1-\exp(-\varkappa^2)\right)|\varkappa^{\alpha-2}|\int\limits_{\mathbb{R}^3}\frac{\langle \varkappa, f^{(n)}(\varkappa-\varkappa')\rangle P_\varkappa f^{(n)}(\varkappa')}{|\varkappa-\varkappa'|^{\alpha}|\varkappa'|^{\alpha}}\mathrm{d}\varkappa' \ . \end{aligned}$$

Choose $\Delta^{(n)}$ so that $V^{(n)}\left(\Delta^{(n)}\right)^{(\alpha-2)/2} = a$ where a is an arbitrary constant, for example, $a = 1$. This gives the expression of $\Delta^{(n)}$ through $V^{(n)}$. From the definitions

$$\beta^{(n+1)} = \max_{\varkappa\in\mathbb{R}^3}\left| \exp(-\varkappa^2) f^{(n)}(\varkappa) + \mathrm{i}\left(1-\exp(-\varkappa^2)\right)|\varkappa|^{\alpha-2} \times \int_{\mathbb{R}^3} \frac{\langle \varkappa, f^{(n)}(\varkappa-\varkappa')\rangle P_\varkappa f^{(n)}(\varkappa')}{|\varkappa-\varkappa'|^\alpha |\varkappa'|^\alpha} \mathrm{d}\varkappa' \right| .$$

If in the limit $n \to \infty$ the functions $f^{(n)}$ converge in the uniform metric to a limit then the limiting function f satisfies the following equation:

$$\beta f(\varkappa h) = \exp(-\varkappa^2) f(\varkappa) + \mathrm{i}\left(1-\exp(-\varkappa^2)\right)|\varkappa|^{\alpha-2} \times \int_{\mathbb{R}^3} \frac{\langle \varkappa, f(\varkappa-\varkappa')\rangle P_\varkappa f(\varkappa')}{|\varkappa-\varkappa'|^\alpha |\varkappa'|^\alpha} \mathrm{d}\varkappa' , \quad (20)$$

where

$$\beta = \max_{\varkappa\in\mathbb{R}^3}\left| \exp(-\varkappa^2) f(\varkappa) + \mathrm{i}\left(1-\exp(-\varkappa^2)\right)|\varkappa|^{\alpha-2} \times \int \frac{\langle \varkappa, f(\varkappa-\varkappa')\rangle P_\varkappa f(\varkappa')}{|\varkappa-\varkappa'|^\alpha |\varkappa'|^\alpha} \mathrm{d}\varkappa' \right| .$$

The value of h is found from the relation:

$$h = \lim_{n\to\infty} \sqrt{\frac{\Delta^{(n+1)}}{\Delta^{(n)}}} = \lim_{n\to\infty} \left(\frac{V^{(n)}}{V^{(n+1)}}\right)^{1/(\alpha-2)} = \lim_{n\to\infty} \beta_n^{-1/(\alpha-2)} = \beta^{-1/(\alpha-2)} .$$

The equation (20) can be considered as the equation for the fixed point of a renormalization group. We are interested only in solutions for which $\beta > 1$. Also the space of odd functions is invariant under the non-linear transformation in the rhs of (20). Therefore the simplest fixed point can be from this subspace. For bounded f the integral

$$\int \frac{\langle \varkappa, f(\varkappa-\varkappa')\rangle P_\varkappa f(\varkappa')}{|\varkappa-\varkappa'|^\alpha |\varkappa'|^\alpha} \mathrm{d}\varkappa'$$

behaves as an homogenous function of degree $4-2\alpha$. Therefore for $\varkappa \to 0$ the non-linear term in (20) decays as $|\varkappa|^{4-\alpha}$. For $\varkappa \to \infty$ it decays as $|\varkappa|^{2-\alpha}$ and it is natural to consider (20) in the space of functions with this type of decay. This scenario of blow-up assumes strong connection between the behavior of initial conditions near $\varkappa = 0$ and $\varkappa = \infty$. We hope to discuss the main equation, its solution, the role of parameter a and the relation t o blow-ups in another paper.

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Analysis on Lie Groups: An Overview of Some Recent Developments and Future Prospects

Nicholas Th. Varopoulos

Université Pierre & Marie Curie – Paris VI & Institut Universitaire de France, Département de Mathématiques, 75252 Paris Cedex 05, France vnth2003@yahoo.ca

1 Introduction

In this paper I want to present some typical recent results in the subject to the general public. A serious effort has been made to make this paper accessible to the nonexpert. The only prerequisite is the definition of a Lie group and its Haar measure, and of the convolution product. Even the definition of the Lie algebra will not be essential and it will be given in Sect. 3 below. Some specialized notions, such as the semigroup $T_t = \mathrm{e}^{-t\Delta}$ generated by the closure of a subelliptic operator $\Delta = -\sum X_j^2$, where X_j are left-invariant vector fields on the real connected Lie group G (the letter G will be reserved throughout to denote such a group), will crop up. The nonspecialist can ignore these, or any other unknown word for that matter, and simply read on, this paper is so structured that this is possible.

The heart of the matter lies in Sect. 2.2 below, Sect. 4 makes comments on the previous sections and Sect. 5 gives some further results. There were several possibilities for the *further results* presented in Sect. 5. My choice was dictated by the following two considerations. On one hand I wanted to present some natural problems in the subject that sooner or later will have to be addressed and which I am sure, have a satisfactory answer. On the other hand I wanted to highlight some much more speculative prospects that emerge from the results presented here. These “speculations” have to do with combinatorial group theory.

Convention

I use throughout the convention that, in a formula, the letters C or c, possibly with suffixes, indicate, possibly different, positive constants that are independent of the important parameters of the formula.

2 The Analysis and the Geometry

2.1 Riemannian Structures on a Lie Group G

For every prescribed inner product $\langle\,\cdot\,,\,\cdot\,\rangle$ on the tangent space $T_e(G)$, where $e \in G$ is the neutral element of G, we can define a left invariant Riemannian structure on G, simply by left translating $(L_g : x \longmapsto gx)$ $\langle\,\cdot\,,\,\cdot\,\rangle$ to an inner product on $T_g(G)$ $(g \in G)$. A different inner product $\langle\,\cdot\,,\,\cdot\,\rangle^{\mathrm{new}}$ gives rise to a new Riemannian structure that is *quasi-isometric* to the initial one in the sense that:

$$C^{-1}|x|^{\mathrm{old}} \leq |x|^{\mathrm{new}} \leq C|x|^{\mathrm{old}}\,, \qquad \forall x \in G\,,$$

where $|x| = d(x,e)$ denotes the Riemannian distance to the origin.

2.2 Convolution Powers

Let $\mu \in \mathbb{P}(G)$ be some probability measure on G, with continuous and compactly supported density $\varphi \in C_0(G)$ with respect to the right Haar measure $\mathrm{d}^r x$ on G: $\mathrm{d}\mu(x) = \varphi(x)\mathrm{d}^r x$. We introduce the following notation, for any integer $n \geq 1$:

$$\mu^{*n} = \mu * \cdots * \mu \quad (n \text{ times})\,, \quad \mathrm{d}\mu^{*n}(x) = \varphi_n(x)\mathrm{d}^r x\,,$$
$$\text{and} \quad \Phi(n) = \Phi(n; G, \mu) = \varphi_n(e)\,.$$

To avoid the obvious pathology (e.g. $G = \mathbb{R}$, $\operatorname{supp}\mu \subset$ positive axis with $\Phi(n) \equiv 0\ \forall n \geq 0$), we shall suppose that μ is *symmetric* i.e. $\mathrm{d}\mu(x^{-1}) = \mathrm{d}\mu(x)$.

2.3 Spectral Gap and Amenability

I shall denote $\|\mu\|_{\mathrm{op}}$ $(\mu \in \mathbb{P}(G))$ the $L^2 \to L^2$ operator norm of $f \longmapsto f * \mu$ on $L^2(G, \mathrm{d}^r x)$ and define $\lambda = \lambda(G,\mu)$ by $\mathrm{e}^{-\lambda} = \|\mu\|_{\mathrm{op}}$. It is important to recall that, for G fixed, either $\lambda(G,\mu) = 0$ for all $\mu \in \mathbb{P}(G)$ as above, and then we say that G is *amenable*, or $\lambda(G,\mu) > 0$ for all $\mu \in \mathbb{P}(G)$ as above, and then we say that G is *not amenable* (cf. [11]).

2.4 Basic Analytic Definitions [16]

We shall say that G is a *B–group* if, for all $\mu \in \mathbb{P}(G)$ and $\lambda = \lambda(G,\mu)$ as in Sect. 2.2 and Sect. 2.3, there exist $C_1, C_2, c_1, c_2 > 0$ such that:

$$C_2 \exp(-\lambda n - c_2 n^{1/3}) \leq \Phi(n) \leq C_1 \exp(-\lambda n - c_1 n^{1/3})\,.$$

We shall say that G is an *NB–group* if, for all $\mu \in \mathbb{P}(G)$ and $\lambda = \lambda(G,\mu)$ as above, there exist $\nu = \nu(G,\mu) \geq 0$ and $C > 0$ such that:

$$C^{-1} n^{-\nu} \mathrm{e}^{-\lambda n} \leq \Phi(n) \leq C n^{-\nu} \mathrm{e}^{-\lambda n}\,.$$

2.5 The Basic Geometric Definition ([4], [18])

We shall say that G (here G is equipped with a Riemannian structure as in Sect. 2.1) admits the *polynomial homotopy property* (*PHP* in short) if the following holds: Let $2 \leq n \leq \dim G$, let $\alpha : \dot{e}^n = S^{n-1} \longrightarrow G$ be some C^∞ mapping of the unit Euclidean sphere into G ($\dot{e}^n$ stands for the boundary of the unit Euclidean n – cell e^n) and let us assume that $\alpha(\dot{e}^n)$ is *homotopic to zero* in G i.e. that α extends to a continuous mapping $\widehat{\alpha} : e^n \longrightarrow G$ (which simply means that $[\alpha]$ is zero in the $(n-1)^{\text{th}}$ homotopy group $\pi_{n-1}(G)$ of G [6]). Then the extension $\widehat{\alpha} : e^n \longrightarrow G$ can be chosen in order that

$$\mathrm{Vol}_n\big[\widehat{\alpha}(e^n)\big] \leq C\big(1 + \mathrm{Vol}_{n-1}\big[\alpha(\dot{e}^n)\big]\big)^c ,$$

for some positive constants C and c depending only on G.

$\mathrm{Vol}_r(\cdot)$ denotes here the r–dimensional Hausdorff measure with respect to the Riemannian structure (counted with multiplicity, cf. [10]). Observe that the above conditions are vacuous if $\dim G = 1$ and that then G admits the *PHP*.

2.6 The Classification: Analytic–Geometric

Theorem A–G. *A group G as above is a* B–group*, resp. an* NB–group *if and only G does not, resp. does admit the* PHP*.*

The above definitions and results extend to measures $\mu \in \mathbb{P}(G)$ that are symmetric but not necessarily compactly supported, provided that they satisfy Gaussian estimates at infinity, which amount grosso modo to imposing $\mu\{x \in G \mid |x| \geq R\} = \mathrm{O}\big(\mathrm{e}^{-cR^2}\big)$ (cf. [16], [19] for the exact definition). The importance of these Gaussian measures lies in the fact that the heat diffusion kernel of the semigroup $T_t = \mathrm{e}^{-t\Delta}$ (cf. Sect. 1) is Gaussian (cf. [16], [22]).

3 The Algebra

3.1 Review of Lie Algebra and Definitions ([9], [12])

Let $\mathfrak{g} = T_e(G)$ be the (real) Lie algebra of G. Recall that every vector $\xi \in T_e(G)$ extends by left translations (cf. Sect. 2.1) to a (left invariant) vector field X on G:

$$X(x) = (\mathrm{d}_e L_x)(\xi) ,$$

and that the Lie bracket on $\mathfrak{g}$ is induced by the bracket of vector fields, viewed as first order differential operators:

$$[\xi_1, \xi_2] = [X_1, X_2](e) = (X_1 \circ X_2 - X_2 \circ X_1)\big|_{x=e} .$$

Recall furthermore that $\mathfrak{g}_{\mathbb{C}} = \mathfrak{g} \otimes \mathbb{C}$ denotes the complexified Lie algebra and

$$\mathrm{ad} : \mathfrak{g}_{(\mathbb{C})} \longrightarrow \mathcal{L}(\mathfrak{g}_{(\mathbb{C})})$$

the (*complexified*) *adjoint representation*, defined by $(\mathrm{ad}\,\xi)(\zeta) = [\xi, \zeta]$. The Lie algebra $\mathfrak{g}$ is *solvable* if the complexified adjoint representation can be simultaneously *triangularized*:

$$\mathrm{ad}\,\xi = \begin{pmatrix} \lambda_1(\xi) & & \star \\ & \ddots & \\ 0 & & \lambda_n(\xi) \end{pmatrix} .$$

Let us decompose $\lambda_j = \mathrm{Re}\,\lambda_j + \mathrm{i}\,\mathrm{Im}\,\lambda_j \in \mathfrak{g}^*_{\mathbb{C}} = \mathfrak{g}^* + \mathrm{i}\mathfrak{g}^*$ and let us consider the (possibly empty) subset $\Lambda = \{L_1, \ldots, L_k\}$ of $\mathfrak{g}^*$, consisting of all distinct $\mathrm{Re}\,\lambda_j \neq 0$.

3.2 The Algebraic Definition (Solvable Case) ([13], [18])

Let $\mathfrak{q}$ be some solvable real Lie algebra and let $\Lambda = \{L_1, \ldots, L_k\} \subset \mathfrak{q}^*$ be as above. We then say that $\mathfrak{q}$ is a *C–algebra* (*C* originally stands for *Condition*) if Λ is not empty and if its convex hull contains 0. We say that $\mathfrak{q}$ is *NC* (*Non–C*) otherwise.

3.3 Review of the Structure of Lie Groups ([7], [12])

It is the fundamental theorem in Lie theory that every real Lie algebra $\mathfrak{g}$ is the Lie algebra of a unique (up to isomorphism) simply connected real Lie group G. Furthermore every Lie group whose Lie algebra is isomorphic to $\mathfrak{g}$ is *locally isomorphic* to G. One basic but standard fact in that direction is that if $\mathfrak{g}$ is solvable then the corresponding simply connected group G is diffeomorphic to $\mathbb{R}^d$.

What is also standard is the following structure theorem: Let G be some simply connected real Lie group. Then

$$G = QK , \tag{1}$$

where Q and K are simply connected closed subgroups of G such that

(i) $Q \cap K = \{e\}$,
(ii) Q is solvable,
(iii) K contains a cocompact discrete closed subgroup Z which is central in G (*cocompact* meaning that K/Z is compact).

Remark 3.1. If G is amenable, Q is the radical and (1) is the Levi decomposition. If G is semisimple, then $Q = NA$ in the Iwasawa decomposition $G = NAK$. Unless G is amenable, Q cannot be normal and in general (1) is related to the Borel decomposition for algebraic groups [8].

3.4 The Algebraic Definition (General Case) [16]

Let $\mathfrak{g}$ be some real Lie algebra, let G_0 be the corresponding simply connected Lie group and let $G_0 = QK$ as in (1) We say that $\mathfrak{g}$ is a *B–algebra* if Q is a C–group. The fact that this definition does not depend on the particular decomposition (1) needs proving. If Q is NC, we say that $\mathfrak{g}$ is *NB* (*B* is the letter preceding *C* in the Latin alphabet and *NB* stands for *Non–B*, and not for the initials in the Greek alphabet of $N.B\alpha\rho o\pi o\upsilon\lambda os$!). For any connected Lie group we say that G is algebraically B (resp. NB) if its Lie algebra is a B (resp. NB) algebra.

Example 3.2. All semisimple Lie groups, compact or not, are NB.

3.5 The Classification: Analytic–Algebraic

Theorem A–A. *G is a* B–group*, resp. an* NB–group *if and only if it is* algebraically–B*, resp.* algebraically–NB*.*

4 Comments

4.1 Unimodular Groups

When G is unimodular i.e. when the Haar measure on G is both left and right invariant, a different classification on the basis of $\Phi(n)$ was carried out in the 80's (cf. [22]). What is involved there are not homotopy considerations but the volume growth of G:

$$\gamma(n) = \text{Haar measure of a ball of radius } n \geq 1 \text{ in } G\,.$$

What we can say then is that when $\gamma(n) \approx n^D$ $(D = 0, 1, \dots)$ we have $\Phi(n) \approx n^{-D/2}$ and when $\gamma(n) \gtrsim n^a$ (for all $a \geq 0$) we have $\Phi(n) \leq \exp(-cn^{1/3})$.

This is a much coarser classification than the one we have here but it has the advantage that it generalizes to all the compactly generated locally compact groups, connected or not.

In terms of our classification given here, the unimodular NB–groups have the additional property that $\nu = \nu(G) \in \frac{1}{2}\mathbb{Z}$ i.e. $\nu = \nu(G)$ is a half integer which depends only on G and not on μ (cf. [14], [17] for a formula that gives ν; cf. [3], [22] for proofs of this when G is respectively semisimple or amenable).

4.2 The State of the Art on Theorem A–A

A complete proof of Theorem A–A when G is amenable can be found in [13]. In [16] one finds a proof for general groups of a slightly weaker result where the NB–condition in Sect. 2.2 is replaced by $C^{-1}\mathrm{e}^{-\lambda n}n^{-\nu_1} \leq \Phi(n) \leq C\mathrm{e}^{-\lambda n}n^{-\nu_2}$. To prove that $\nu_1 = \nu_2$ and to compute this index is a truly formidable task, and it takes from end to end several hundred pages to carry out. The reason is that, among other things, the solution of that problem relies on difficult estimates in potential theory (cf. [21]). It is a fortunate fact that these potential theoretic estimates have, very recently, come on their own and have given rise to interesting new results in classical probability (and potential) theory. Let me explain.

Let $\mu \in \mathbb{P}(\mathbb{R}^d)$ be some centered probability distribution with a high enough moment, and let $D = \{x = (x_1, x') \in \mathbb{R}^d = \mathbb{R} \times \mathbb{R}^{d-1} \mid x_1 > \varphi(x')\}$ be some Lipschitz domain in $\mathbb{R}^d$, where $|\varphi(x') - \varphi(y')| \leq A|x' - y'|$ $(x', y' \in \mathbb{R}^{d-1})$. Let

$$P(n, x) = \mathbb{P}_x[Z_j \in D; j = 1, 2, \ldots, n]$$

be the probability of life (or the gambler's ruin estimate, depending on the point of view) of the random walk $Z_1, Z_2, \dots \in \mathbb{R}^d$ controlled by μ, i.e.:

$$\mathbb{P}[Z_{n+1} \in \mathrm{d}y // Z_n = x] = \mathrm{d}\mu(x - y) , \qquad x, y \in \mathbb{R}^d,\ n = 0, 1, 2, \ldots .$$

Very precise estimates of $P(n, x)$ can be obtained in the above generality (cf. [21]). These estimates are essential for Theorem A–A, where D is then an appropriate conical domain in $\mathfrak{g}$ $(= \mathbb{R}^d$ as a linear space) defined by the positivity of the relevant roots (i.e. D is a generalized *Weyl chamber* [5], [13]).

Be that as it may, the complete proof of Theorem A–A will appear in a forthcoming paper [20].

4.3 The State of the Art on Theorem A–G

In [18] one finds a proof, among other things, of Theorem A–G when G is solvable and simply connected. What allows one to pass to a general connected Lie group G is that, if $T \subset G$ denotes the maximal normal torus of G, then $G/T \simeq Q \times K$ is quasi-isometrically diffeomorphic (but not necessarily homeomorphic) to the product of a simply connected solvable group Q and of a compact group K (cf. [18]; the proof of this is not difficult and it will appear in [20]). This allows us to reduce the problem to compact groups and what has to be proved is that every connected compact group admits the PHP.

I claim to have a proof of this fact on compact groups (which is quite involved). This is in the spirit of differential topology and Morse theory. The details of this have not yet been written out in full and, since in addition I am not an expert in differential topology, I feel that I have to warn the reader that unpleasant surprises in that direction are not to be excluded altogether (in plain terms my proof might collapse). Even without the above result for compact groups however, the results of [18] give a, perhaps less elegant to describe, but equally pertinent, B–NB geometric classification of Lie groups.

What emerges also from the results of [18] is a cohomological classification of Lie groups. (These results have been stated precisely in [18] but the proofs remain to be written out. These proofs are however easy to extract from [18].) Grosso modo, let us say that G, equipped with a Riemannian structure as in Sect. 2.1, has the *cohomological polynomial property* if, for every smooth differential form $\omega \in \wedge(G)$ that *grows polynomially* at infinity (cf. [18] for precise statements), that is closed (i.e. $\mathrm{d}\omega = 0$), and that represents the zero cohomology class of G, we can find $\theta \in \wedge(G)$, also with polynomial growth at infinity, such that $\mathrm{d}\theta = \omega$. The cohomological classification of Lie groups states then that G is an NB–group if and only if it has the polynomial cohomology property.

5 Further Results and Prospects

5.1 A Direct Proof of Theorem A–G

The most significant progress in the direction that I described in the previous sections would be to give a "direct" proof of Theorem A–G. By this I mean a proof that does not use the Algebraic classification of Sect. 3.2. This should be done in the spirit of [22] where in fact the above task is carried out for unimodular amenable G.

The reason why such a project is significant is that there would then be hope to extend the result to discrete groups. I shall discuss the problem of discrete groups in Sect. 5.2 below. But before I do that I wish to put the above project in perspective by considering another closely related, better posed, but also less interesting problem.

Let Q be some simply connected soluble Lie Group and let use assume that it is possible to assign such a group with a left invariant Riemannian structure with non positive curvature (necessary and sufficient conditions on the Lie Algebra for this to be possible exist [1]). We can then use the Geodesic Flow to show that then Q admits the PHP and even obtain optimal estimates in the definition e.g. for $n = 2$ in Sect. 2.5 we have

$$\mathrm{Vol}_2[\hat{\alpha}(e^2)] \ \leq C(1 + \mathrm{Vol}_1[\alpha(\dot{e}^2)])^2$$

and analogous results for every homotopy group π_n.

It is very likely and probably not even very hard to adapt [18] and go again via the Lie Algebra to show that the above optimal estimates on the volumes of the π_n's can be used to characterize the negatively curved groups Q.

Question 5.1. First of all is the above correct?

Question 5.2. If so, can one give a direct proof without going through [1]?

The interest of the above is that it would perhaps give some clue of how to go about a direct proof of the Theorem A–G.

5.2 Combinatorial Group Theory [2]

Let G be a finitely presented discrete group. We can glue to the Cayley graph of G associated to the generators, the 2–cells that correspond to the relations, and obtain thus a 2–dimensional G invariant CW–complex. 1–dim and 2–dim Hausdorff measures that are G invariant can clearly be assigned and the PHP for dimension $n = 2$ of Sect. 2.5 can clearly be defined. Analogous definitions for $n \geq 2$ can also be given, and all in all, the statement of Theorem A–G "makes sense".

Question 5.3. The issue is to decide if such a theorem in some appropriate form is provable?

The importance of the above PHP adapted to discrete groups has been recently stressed by several authors (e.g.[4]), and of course it can be restated and it gives an equivalent description of the word problem.

Example 5.4. Let $G = \pi_1(K)$ where K is a negatively curved compact manifold be a hyperbolic group. We can use then the geodesic flow on the universal cover $\tilde{K}$ to generate the homotopy and obtain the so called Dehn algorithm for the word problem.

5.3 More Concrete Problems

The project that I described in Sects. 5.1 and 5.2 may well be "daydreaming". There certainly does not seem to be much lead of how to start.

A much more realistic project, but also much more esoteric, is to examine in more detail the "polynomial property" of the various dimensions $n = 2, \cdots$, for the homotopies of Sect. 2.5 or the cohomologies of Sect. 4.3. Some dimensions may have the polynomial property and others not. Many examples can be given of all short of situations [4] [18]. A complete classification in terms of the GL_k–geometry (cf. Sect. 3.2) of the roots (like the C–condition but more refined) is no doubt within reach. Let us assume that we can write down such a classification. The question then arises whether we can read off these properties in terms of "Analytic" or rather Potential theoretic conditions as in Sect. 2.4? In other words:

Question 5.5. Can we refine Theorem A–G in terms of the polynomial behaviour of the "various homotopy groups $\pi_n(G)$"?

This also would be a first step towards the speculations of Sect. 5.1. But even here it is hard to make the right conjectures.

Observe that in Sect. 5.2 it is not the discreetness of the groups G that is the problem it is the lack of the Lie algebra. So we could simplify G and assume that it is, say, a cocompact lattice in some (non compact) semi-simple Lie group. What can we say about $\Phi(n, \mu)$ of Sects. 2.2 and 2.3 then. For instance:

Question 5.6. Can we assert, that $\Phi(n) \sim n^{-\alpha} e^{\lambda n}$ (cf. Sect. 4.1) where $\lambda > 0$ will have to depend on μ but $\alpha = \alpha(G)$ is a genuine group invariant?

This is what happens for the semi-simple Lie group itself [3]. The above is a concrete problem and it is probably within reach (there was a point that I even thought I could prove this. I have since drifted away from the subject and now I do not know any more). Problems like this may have an arithmetic significance. I am however very ignorant on arithmetic questions and any comment from me in that direction would be inappropriate.

5.4 Hardy–Littlewood Results ([14], [15])

An interesting direction where the final results remain to be worked out are the $L^p \to L^q$ mapping properties of

$$\Delta^{-\alpha/2} = \frac{1}{\Gamma(\alpha/2)} \int_0^\infty t^{\alpha/2-1} T_t \mathrm{d}t \,, \tag{2}$$

where $\alpha > 0$ and $1 \leq p < q < +\infty$. Here I use the semigroup Laplace transform definition of the fractional powers of the Laplacian, and the notation of Sect. 1. Fairly satisfactory general results in that direction only exist in the unimodular case (cf. [14], [22]). What renders the above problem difficult is that the range of parameters (α, p, q), for which $\Delta^{-\alpha/2} : L^p \longrightarrow L^q$, depends in general (if G is not unimodular) on the particular Laplacian Δ and does not only depend on G (just as the $\nu(G, \mu)$ in Sect. 3 depends in general on μ).

A moment's reflexion shows that, for *amenable* groups, what is relevant for (2) are the following parameters:

$$\begin{aligned}
\mathrm{d}^\ell x &= \text{left Haar measure} \,, & m(x) &= \frac{\mathrm{d}^r x}{\mathrm{d}^\ell x} \,, \\
\widetilde{T}_t &= m^{1/2} \circ T_t \circ m^{-1/2} \,, & \ell(q) &= \overline{\lim_{t\to\infty}} \frac{1}{t} \log \|\widetilde{T}_t\|_{1\to q} \,, \\
L &= \inf\{q \geq 1 \mid \ell(q) = 0\} \,,
\end{aligned}$$

where we take here the $L^1 \to L^q$ operator norm w.r.t. $\mathrm{d}^\ell x$, and where we have to consider here $\widetilde{T}_t$, because the original semigroup T_t (cf. Sect. 1) is not symmetric. L is the *cut point* between the exponential and the subexponential growth of $\|\widetilde{T}_t\|_{1\to q}$ and it is easy to see that $1 \leq L \leq 2$. The following result is sharp, but unfortunately, very limited in scope and not easy to prove:

Fact 5.7. $L = L(G)$ only depends on G and is independent of the particular laplacian Δ. Furthermore $L = 1$ if and only if G is unimodular and $L = 2$ if and only if G is WNC.

WNC (*Weak–NC*) is a variant of the NB and NC definitions given in Sect. 3 (cf. [15]). The above can be reformulated by saying that, if the operator

(2) with T_t replaced by $\widetilde{T}_t$, is bounded for some $\alpha > 0$ and $1 \leq p < q < 2$, then G is a *WNB–group*. This is very much in the spirit of the results that we expect to hold. Unfortunately what the correct conjectures are, is not clear.

Working out in full generality the above Hardy–Littlewood theory is challenging and, I feel, is within reach. The only problem is that it cannot be done by easy and superficial contributions. It would take a competent man (or woman. Why not !) several years to complete this project. I am probably too old to attempt this, but others should try. Just to qualify this last statement, I could also say that convincing applications, outside the subject itself (e.g. arithmetic results on lattices), would have to exist, before a *competent* man decides to spend several years on such a problem.

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Encounters with Science: Dialogues in Five Parts*

Lars Gårding

University of Lund, Sweden Lars.Garding@math.lu.se

Preface

In our time Science gets its prestige from many successful applications and now cohabits peacefully with religion and philosophy, with political power, with the general public and with the media. In this situation Science appears as a respectable whole and a certain decorum is required to alleviate the fact that science may be very difficult to understand, that scientific work can be dull and insignificant and that many branches of science have very different goals, methods of research and criteria for acceptability.

In the dialogues of Encounters with Science this decorum is broken in all the cases of cohabitation above. The only aim of the author has been to encourage reflection and sometimes to amuse.

The text has five parts. The first is called Mathematics, Life and Death and is a miniature play in two acts about the mathematician John von Neumann's adventures in heaven and hell. In the second part, called Ghosts, Charles Darwin and Henri Poincaré reappear to discuss science after their time. The third part, called the Soul of Science, features Lady Scientia, the guardian spirit of Science, talking to Common Sense represented by Simplicio, a character from Galileo's dialogues. In a rambling encounter they discuss the conflict between common sense and certain parts of physics, applied versus pure science and the recent industrialization of science which puts a great burden on Lady Scientia. In the next dialogue Lady Scientia is free to express her views to the press in an impromptu interview. The definition of the word science is settled in a discussion between two contemporary young students aspiring to their Ph.D's. In a fourth part, entitled The Prince, political power appears in person as the ruler of Syracuse talking to Archimedes and in a dream a

* Lars Gårding was expected to speak at the conference, but unforeseen circumstances arose at the last minute and he was unable to attend. We are pleased to present his contribution, which consists of several dialogues on science and mathematics as well as their interaction with philosophy, religion, and society.

present representative talks to the press about science. The fifth part, Communication, features a duel between science and the humanities, a section on metaphors and a piece on how to appear in the media.

Lund, Sweden, *Lars Gårding*
June 2003

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MATHEMATICS, LIFE AND DEATH I

1 Von Neumann and God

A simple space with a background through which the actors can disappear. A table and two chairs. Characters: von Neumann (N.), a world famous mathematician, God (G.). A conversation in heaven. No music. God is sitting at the table. Von Neumann enters through the curtain.

G. Welcome John von Neumann. Please sit down.

N. Thank you.

G. How are you?

N. Better than when I was in the hospital. And yourself?

G. I am well, thank you. I have decided to be well. I am almighty, you know.

N. Who are you?

G. God.

N. That sounds strange. Tell me more. Might you be the God that is mentioned in the Holy Scriptures?

G. The same. In human form.

N. Then perhaps you know all future mathematics?

G. Yes, but I let mathematics evolve by itself. It is more entertaining that way.

N. What is my work in logic worth? No one quotes me any more.

G. As I said, I let man deal with appreciation and disdain. Here, among us, a higher logic prevails, a logic not accessible to man. I advise you in your new, more tranquil circumstances, to take your time and see what happens among men. If they discover inconsistencies in mathematics, that is their business. One can do no more than regret not being present at such interesting events.

N. My first ambition in life was to make my mark, and then it was a matter of being of use and taking thinking as a diversion. I was never calm and happy.

G. That was never my intention with mankind.

N. I wrote down the axioms for Hilbert space and afterwards I felt them as a constraint. My rings of operators became nothing more than a catalogue of possibilities. I wanted to do something new but I was only partly successful. I intended to create logical system that would cover the activities of the brain, but I did not have time to develop it properly. I was interrupted by my illness. My life ended prematurely If you are who you say you are, then all this is your fault. Why did you not let me live?

G. My omnipotence is often delegated to chance. Otherwise there would be much too much to do. It was chance that you were born and chance that gave you cancer. I watched and did nothing. You understand that I have more to keep an eye on than your affairs.

N. What for instance?

G. Everything that happens, will happen and has happened. The well-being of mankind, the smallest insect and so on.

N. Yet you seem to take things easy.

G. I am dealing with you just now. What are your views on the deepest questions of mathematics?

N. Unlike Wittgenstein for example I have never had a desire to let fundamental questions disturb my peace of mind. In mathematics I am an opportunist. So many wonderful things have been done, and so much has been understood. An occasional philosopher sometimes protests about our way of understanding, but since philosophers question everything one does not have to take much notice of what they say. They never have a proper set of axioms.If mathematics should contain a contradiction it would only be in the outer areas of the subject and could be corrected by small changes. That is my point of view. I am an opportunist. (*pause*)

There is, by the way, something strange about the attraction the so-called ultimate questions hold for people. They know nothing about mathematics, yet they are concerned about the subject's validity. This sometimes takes grotesque forms. My colleague Gödel spent days answering letters about his incompleteness theorem. He had to explain that it did not address eternal truth or the existence of God (you'll excuse me I hope) but a certain way of numbering the propositions in a logical system.

Those who got in touch with him had a fundamental religious longing for a life that was a blessed, eternal holiday. Do you have a comment? You may not be entirely omnipotent, but you seem to think and have opinions. What do you think about mathematics for example.

G. I *am* omnipotent, but as I have already told you I can delegate my omnipotence. One reason for doing so is that I don't want to get into logical difficulties. Total omnipotence means that I should have almighty power over myself, and then I would be both almighty and not almighty. That is a logical paradox that would have incalculable consequences. On this point you as a mathematicians would understand me far better than many others. I must say it feels good to have such a competent partner in conversation. And now, if you will allow me, I shall answer your questions in detail. They relate to matters of great concern to me.

My omnipotence would be heavy burden unless I did not wholly or partly leave it to chance, to the forces of nature, to certain people, writers, artists, scientists and so on. Sometimes even the devil has a part in my omnipotence but, it goes without saying, within certain limits. In other words, sometimes I use my omnipotence, sometimes not. But of course I, myself, decide where and when to use it. Anything else would be unthinkable. I enjoy my freedom, I must say. (*pause*)

You asked about my opinions. Yes, I have opinions or, more precisely, opinions have always been attributed to me. What they are now is in some doubt. It used to be easy: in my opinion man should be honest and upright, attend the services and have an unshakable faith in me and in Holy Scriptures. Now the only people I can really trust in this respect are the Muslims. I see religious life becoming degraded, although the opinion that I exist seems to be fairly solid. But none of this concerns me. People need me, not I them.

Then there is the matter of mathematics. (*solemnly*) He who guides the fate of the world cannot be an opportunist. I believe in a mathematics that is uniform and free of contradiction. But I can tolerate doubt in some people, particularly those you speak disparagingly about. I have sympathy for the uncompromising doubters. I may have them held up and admired for their spiritual attitude to the mysteries of science, life and death. For ever and ever. Amen.

N. Spare me your religious tone. Your way of combining faith and doubt reminds me of the late Wittgenstein. Were you influenced by him?

G. I am not influenced by mortals. On the contrary, they are influenced by me.

N. Let me return to mathematics. Is Riemann's hypothesis true?

G. Yes!

N. Then give me the proof.

G. I see the proof at a glance. It would take too long to translate it into English or Hungarian. You will have to accept that Riemann's hypothesis is true.

N. You must be joking. Give me the proof!

G. I am not joking. If you continue to make trouble I have angels that can carry you to Hell. Do you long to be there?

N. (*agitated*) Give me the proof!

G. You can kick up as much fuss as you please. It doesn't worry me.

N. I must know if you are bluffing or not. Do you understand why quantum mechanics contains so many troublesome infinities?

G. Understand! Of course I understand. When I created quantum mechanics I was not in best form, but it hangs together.

N. Your answer is ridiculous. I find it more and more difficult to believe that you are God.

G. We will not come further with your questions. How do you want your life to be here in My House. Do you want something to do? The position as a heavenly meteorologist perhaps?

N. I should want a closer description, please.

G. Our meteorologists take care of the weather on earth. I employ an angel to pour water on the earth, another one takes care of snow and, sometimes, hail. I have also an enormous angel who blows and cares about the wind. But all these tasks are taken care of. Weather here in heaven is completely predictable and everyone knows how it will be. You could perhaps make it more equal weather on earth. But within limits of course. I offer you this position.

N. I do not want it. Can't I be a mathematician? I am a mathematician.

G. That is impossible. All mathematics here is within me and I never put anything in writing. I have even banned all writing. Everything has to be communicated orally and in small amounts. Heaven could not survive the restless systems that prevail on earth. We must lead ecological lives in the heavenly sense.

N. You are not God. I have heard too many contradictions already. You pretend to understand everything and know everything, yet you have a ridiculous and contradictory system for weather on earth. It is impossible for rain, snow and hail to be arranged as you say. Either you are an impostor, a vulgar impostor, or you are just making fun of me.

G. I am not making fun of you. I am God. Not an impostor. And to show you, I will have it thunder. Go, thunder! (*A terrible noise is heard*) Be careful!

N. You do not scare me. I am leaving. (*Walks away, but bumps into an invisible wall. Tries in vain to find a way out.*)

G. You shall not go away. I will stop you. (*N. Makes further, more half-hearted efforts to leave. Finally he sits down.*)

N. (*somewhat out of breath.*) I still think that you are a fake. Where are your hosts of angels, where is paradise, where are the archangels, where is Gabriel? Where is Jesus? Isn't he supposed to sit at your right hand?

G. Those you seek exist in my head. I myself can see them and hence have them exist whenever I want. People who think of heaven as a copy of earth have no imagination.

N. You make me more and more confused. Where are we?

G. Here, here!

N. Where is here?

G. That is unspecified. Since we are talking so much it is impossible to determine at the same time where we are.

N. Do you refer to the indeterminacy of quantum mechanics?

G. Not exactly, something similar. (*Both are silent for a long time*) Perhaps we should make peace with each other. You like to think. Let us think together.

N. I do not mind. (*Both adopt a thinking pause. There is a long silence.*)

N. What did you think about?

G. Everything, an endless amount.

N. Can't you take something out?

G. I don't want to. It would destroy unity. For me everything hangs together, my thinking is holistic. What have you been thinking about?

N. About primes. Without the prime number structure of the integers Gödel could not have done his numbering.

G. I'm sorry?

N. The integers are 1,2,3,4,5 etc. According to a famous mathematician, Leopold Kronecker, you created them. Is this true?

G. Of course! Please continue!

N. Certain numbers are products of other numbers except the number 1, some do not have this property and they are called primes. For instance: the number twenty which equals five times four is not a prime, neither is four but five is a prime as are two and three. The first primes are 2, 3, 5, 7, 11, 13, 17, 19, 23, ...

G. (*interrupts*) Yes, yes, I see then all: 29, 31, 37, 41, 43, 47, 51 (*a discrete cough from von Neumann*), no that is three times seventeen, 53, 57, no, that is three times nineteen, 61, 67, 71, ... (*This sequence is pronounced more and slowly*).

N. (*interrupts*) Stop! Stop! Your counting will never end. There are infinitely many primes.

G. I know that very well. I see all of them at a glance.

N. This I cannot do. But I can prove that there are infinitely many primes. The method runs as follows. Take any primes, multiply them together and add the number 1. The number that get in this way is either a prime or a product of primes neither of which is a member of the first ones chosen. However many primes that are listed, there is always at least one more.

G. Do not ever lecture me! Use figures!

N. Two times seven is fourteen and fourteen plus one is fifteen. Fifteen is five times three. Simsalabim! Out of the primes two and three the method produced the primes three and five!

G. Very clever. And new to me.

N. The proof is two thousand four hundred years old.

G. But when, like me, one understands and sees everything, proofs are becoming things of secondary interest. Other things take up my time. There are so many services and prayers to hear. I listen a little absent-mindedly but I cannot disregard sometimes fervent prayers. Although I am omnipotent I have to take in consideration people's conceptions of me. I cannot appear to be too stern and forbidding.

N. Your existence and conditions on earth means a contradiction which is usually called the problem of evil. Your are all-wise, all-mighty and all-good.

How does that square with illness, suffering, sin and evil, sudden death on earth?

G. It pleases you to make fun of me. You have seen for yourself that I have threatened you and restricted you against your will. I am not good all through. The one who created the universe and life and death on earth is not good and cannot be good. —— With your mathematical jargon I could say that the problem of evil is wrongly put. Talking of such things I was once much amused by Leibniz's solution of the problem of evil, that man lives in the best of all conceivable worlds. There is only one catch with that. Who is doing the conceiving, he or I?

N. I admire Leibniz as a mathematician, but he was above all a philosopher. What are your thoughts about philosophy?

G. I have nothing against philosophy except that it is sometimes very tiring. But not dull! I must say that philosophers with a strong faith who have not questioned my wisdom or omnipotence have often performed interesting pirouettes in their thinking. But in the end they had to allow unproven ideas to avoid conflict with the human reason. Divine reason sees no such limitations. For me it is the question of seeing the whole picture and not getting caught up in details. By creating reality I gave the philosophical concept of reality a meaningful content. And if one keeps to existence all logical problems disappear.

N. Your own existence is a logical problem. If you are part of reality you exist and if you are not part of reality you do not exist. Since you created reality and existence you cannot yourself exist provided you have some kind of identity. It is not true that all problems disappear if one keeps to existence.

G. I exist, that is obvious. And I have not created myself. I'll have no hair-splitting here, please!

N. The inescapable conclusion of you having created existence is that you do not exist. And if you exist you have not created existence.

G. But I am sitting here and you see that I exist. And I created everything!

N. You do not want to understand. But I still keep my human reason. Is that some oversight on your part?

G. Not at all. In fact, man's struggle with logic amuses me.

N. But it does not amuse me to play a kind of clown for you. I have thoughts of my own that you cannot see through.

G. God forbid! But I am a little uncertain.

N. Let us abandon philosophy and pass to mechanics? Are you conscious of the sun, the planets and the comets?

G. This is the second time that you are trying to make fun of me. There is only one answer to your impertinent question: of course!

N. Do you remember how it was like to create the solar system?

G. Remember! For me time and space are no boundaries. At the creation I said ‘Let there be light’ and then on the third day or perhaps the second the solar system came into being when I created the large heavenly lights. I said ‘Let there be the sun and moon and stars’. Genesis does not say much more but I have always thought that this book is too short to do me justice. I remember for sure that I also created the lesser but moveable heavenly lights. I said ‘Let there be planets’. Then I could see everything from my elevated vantage point. How the earth and the planets move among themselves, around the sun and around me. It was a grand spectacle. I changed nothing because I thought the result good.

N. How about gravitation?

G. What do you mean? You speak in riddles.

N. The rotation of planets around the sun follows from the principle of gravitation. In the mathematical model for the planetary system it is assumed that two point masses are attracted to each other by a force that is proportional to the product of their masses and inversely proportional to the square of the distance between them. This law and the principle of acceleration determine the future movements of any number of such masses when their positions and velocities are given at some point in time.

G. This sounds good, but what is mass and so on.

N. That can be explained but the point is that the movements of a planetary system can be summarized and explained by a simple mathematical model. You said ‘Let there be so and so’ and the result is governed by a simple principle.

G. I could understand what you just said if I wanted. I am not stupid, you know. But I am more surprised than interested. Did you find all this out?

N. No, the culprit is Isaac Newton three hundred years ago.

G. Well, well,... Now I remember. The philosophers made me a clock maker who created a mechanical universe that goes by itself. That was an insult!

N. Gravitation made it possible to understand the movements of the planetary system. And this was tremendous success for theoretical physics. And Einstein’s relativity theory made it even better. It cannot be formulated as cause and effect, only as a variational principle. I, and many with me, consider variational principles to be the innermost foundation of the universe. What is your opinion? Do you have one?

G. Maybe, but please realize that I understand *everything* and need not reveal anything. Too much science disturbs the harmony of the universe.

N. You say that you understand, but what is meant by understanding?

G. To see without details is the Almighty’s way of understanding.

N. (*ironically*) Brilliant? Perhaps you can teach me to understand in this excellent way?

G. I warn you. Irony has no place in heaven.

N. (*still ironic*) Why did you not make the creation more systematic and scientific. You could have started with the chemical elements. You could have said 'Let there be Helium, let there be Lithium, let there be Beryllium, let there be Boron, let there be Carbon' and so on. Or in order not to be long-winded you could have said simply 'Let there be a Bang'.

G. I'm sorry?

N. According to one theory the universe was created in 3 seconds from concentrated energy by an explosive expansion, jokingly referred to as the Big Bang. The chemical elements were formed as well as nebulae, milky ways and so on. Universe as we see it now.

G. You are beginning to go too far. Finding fault with me about the creation! If things were as you say, I was the Big Bang. But creation has to be understood by people without education. So I chose to begin by floating above the waters and speaking in pictures to man in man's way.

N. (*seriously*) You are wrong to place rhetoric over science. Mathematical models are the best way to understand nature. Such models are especially sharp and completely successful in many important cases. But that doesn't mean that they cannot fail or be applied badly. All of them were created by man.

G. Ahh, now you are not so sure!

N. (*enthusiastically*) Our knowledge is temporary but sure in important areas. Relativity theory, quantum mechanics, light and electricity have been combined into a wonderful unit whose predictions have been verified a thousand times by experiment. We are on our way towards understanding the structure of matter. What is still missing is a theory that includes gravitation also. (*ironically*) But you who are omnipotent and knows everything, you could perhaps help us?

G. I will not hear your prayers. The answer is no.

N. Why?

G. It is very rarely that I motivate my nos. But now I will make an exception. I created man and I am loyal to him. What you speak about is understood by a very small minority. I must be understood by many and look after so many details, both small and large, precise and random, that I have no time for mathematical models. At best as a pastime. Philosophy as a hobby. The welfare of man is my major task. My view is holistic.

N. (*furiously*). You say that you understand but now it is I who really understand what is happening. In our conversation you have tried to adjust to me. You have pretended to understand and always replied to me in everyday language.

At the same time you have no idea of the laws of nature that govern both you and all others. And you also pretend that man's welfare is your main task. Incredible. Everyone suffers and dies under your welfare and, like me, most people die too soon and in terrible fear. Your omnipotence is an illusion without substance. Your Heaven is a quiet Hell, a reflection of a more interesting hell on earth.

But you have no intellect. You simply mirror the person who is talking to you. You believe that you are God, but you are an apathetic witness to the miracles of nature and life. Man created you. It is men's desires and fears that are portrayed in you. The result is difficult to tell apart from another figure. I mean the Devil.

G. (*calmly*) You blaspheme and that is no good to either one of us. Our conversation has not been uninteresting but now it is finished. (*G. disappears into the background by a light effect. N. Is left alone and waits for a long time, mumbling and gesturing in a way that first expresses fury and triumph and then doubt. Finally a voice is heard: 'John von Neumann is granted an audience with the Devil.'*

Curtain

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MATHEMATICS, LIFE AND DEATH II

2 With the Devil

Same scenery as in Act 1 with a table and two chairs but no curtain of light. A dark backdrop from which the actors come and go. The actor who played God can play the Devil. Characters: von Neumann (N), the Devil (D), Immanuel Kant (K), David Hume (H), Aurelius Augustinus (St. Augustin) (A).[2] *D sits alone by the table, N enters.*

D. Please be seated.

N. Thank you (*sits down*).

D. How are you?

N. I was very excited but now I have calmed down. Who are you?

D. I am the Devil himself.

N. How am I to know that?

D. You have to believe me. (*Thunder is heard*). Up there HE is trying to prove his identity. I can't use the same means. Only a round trip in Hell could convince you, but we have a lot to talk about before it is time for that. Of course I know that HE sent you here.

N. Not directly. God disappeared and then someone called out that I had to go to the Devil.

D. Everything happens by HIS will. Most people come here directly. A detour via Heaven is actually very rare. I am supposed to have been there before the Fall but total oblivion was part of my punishment. So I have no memories of the place. I hope you excuse me if I now ask you some questions. What is it like in Heaven?.

N. I do not know. I had a conversation with someone who said he was God. This might even have been the case but not in the way that he thought.

D. But how was it? How did it all look? Was it hot or cold, were the streets paved with gold and did you hear singing and dancing day and night?

N. I sat at a table, about the same as this one. I was prevented from going away. When I asked him about Jesus and the angels he said he had them in his head.

D. It is clear that you have seen very little.

N. God lives in an illusion of omnipotence. He says that he extends it over you.

D. Unfortunately.

[2] A.'s polemics against the Pelagians is used in the conversation between A and N

N. When I accused God of being a phantom created by human yearning and fright he disappeared and I woke up here. Are you also going to leave me?

D. No, never. I have to arrange things for you. Do you have any wishes?

N. I would prefer a quiet existence where I can think about mathematics.

D. Existence!? For you existence is finished.

N. I do not believe you. In your house small devils torment small sinners with tongs and the greater ones are burning for ever.

D. There may be some truth in that but here with us there is no time and without time there is no existence. Everything here goes back and forth in time. Everything happens both simultaneously and not simultaneously. It is this that makes Hell what it is.

N. If you can make time go backwards, you can perhaps arrange for me to be born again. On earth of course.

D. This is impossible. Such power is out of the question for me. Time order cannot be controlled.

N. If time order is indeterminate, what about logic and mathematics? Are they possible in hell?

D. Not entirely, it is only the law of cause and effect that ceases to have a meaning...

N. But we are engaged in a normal conversation taking turns to speak?

D. This can only happen in Hell's ante-chamber where we are now.

N. Let me never leave this place.

D. This is impossible. I must lead you further on into Hell.

N. What are my prospects? If prospects exist here of course.

D. So far you have one thing to do. To talk to interesting persons. You are even sought after. HE has spoken to you and therefore many people want to air their thoughts with you. Rumours of your conversation with HIM are widespread. And we have many interesting characters in Hell's antechamber. Some are here for ever, others who have tired of the other place are here for shorter or longer periods. A kind of vacation you might say. Whom do you want to see? Here in Hell we use telepathy to make people meet and exchange views. I hear that Immanuel Kant wants to talk with you. Heaven disapproved of the tone of his philosophy and that is why he is a permanent guest here in the antechamber of Hell. He did not go further since his life was without reproach. Ah, here he comes. (*N. rises*)

K. A good day to you, Professor von Neumann, it pleases me to be able to talk to such a prominent mathematician. May I first ask you not to bring up the phrase 'Das Ding an sich' in our conversation. I write in my book that this notion is meaningless but this has not prevented philosophers from forever asking what I mean by it. Unfortunately I cannot prevent them (*makes gesture*).

The foundation of my philosophy is that all search for truth must depart from some basic assumptions, or, to use your language, axioms. Otherwise one is lost in a mire of senselessness.

N. I agree with you completely.

K. Could you please be kind enough to explain to me Gödel's theory of undecidable propositions. Here I only hear unreliable rumors and, so far, I have not had the pleasure of meeting Professor Gödel personally.

N. In your own treatise *Kritik der reinen Vernunft* there are four antinomies...

K. (*intercedes, speaks slowly in a professorial manner*) Of course, in the first one, two opposite theses are proved, namely that the universe has a beginning and is finite in extent and, the opposite one, that universe has always existed and extends indefinitely. In the second antinomy I proved that everything is composed of simple parts and also that everything is not composed of simple parts. In the third antinomy it is proved and disproved that everything happens according to the laws of nature and, finally, the fourth antinomy proves and disproves that there is a being which is the cause of everything that exists or happens. All this of course with the greatest brevity. As I say in the book, all proofs are conducted with the utmost care and in the greatest possible respect for the truth.

N. This I do not doubt. In our time your proofs would have been more formal but with no essential changes. The answer to your question is now simple: Gödel's theorem says that every complete logical system must contain at least one antinomy.

K. And what is a complete formal logical system?

N. Like geometry. One proceeds with axioms and logic and leaves nothing out.

K. That was an excellent answer. I am very grateful.

N. I believe that our ways of thinking agree in other ways. Do you not agree that one has to distinguish between reality and thoughts about reality?

K. (*Enthusiastically*) This is my great discovery and my consolation now that I am condemned to the antechamber of Hell.

N. I believe that God is created by the thoughts of humans, by their fright and yearning.

K. I could not go that far. I lived in another time. But let me embrace you. (*K. and N. embrace, exit K.*)

D. A pity that you two finished. Your conversation started off well and lasted long. But look, here is David Hume.

H. I can only regret that Herr Kant was after my time. If we only had been contemporaries, I could have disproved his Prussian phantasies and rejected them with great force. (*Turns to N.*) Who are you?

N. John von Neumann, 1903–57, mathematician.

H. Since I reject the existence of the outer world you simply cannot exist as a philosophical subject.

N. Very interesting. When I proved to God that he does not exist he answered me very simply. He said: But I am sitting here. I can answer you in the same way: I am standing here.

H. This is because I am looking at you. If I turn another way, your existence ceases.

N. But there are so many viewers. Hence everything oscillates between existence and non-existence in an uncontrollable way. Things are and they are not.

H. This is an inescapable consequence of my theory. It could be possible that God sees everything and this gives existence a certain permanence. But this argument belongs to the advanced parts of my philosophy. Anyway, you bother me. What are your credentials?

N. My mathematical theorems are well known and they are used every day.

H. But I do not see them and hence they do not exist.

N. But, Mr. Hume, mathematical theorems do not form a part of reality. They belong to thought and those who use them give them life by thinking.

H. Things are real only through a viewer. That is final.

N. But mathematics is more real than reality. Ideas are more real than reality. As you know very well this was the view of the famous philosopher Plato and it is in fact the cornerstone of his theory.

H. You forget that my philosophy is later than Plato's and hence more true.

N. Maybe you also deny Descartes' famous dictum: I think and hence I exist. In my philosophy I changed this to: I think about something, hence it exists. Besides, I cannot agree with your idea that one philosophy falsifies all earlier ones. If you really accept this as true, all philosophy from the twentieth century is superior to all earlier philosophy including your own.

H. Your philosophy!! Nobody heard of it.

N. This may be true but since I think about my philosophy, it exists. (*A pause*) It would be interesting to hear your views on the law of cause and effect. About this I had a most interesting discussion with Herr Kant.

H. Then you only heard some Prussian nonsense. I see no causes, only extrapolations of observed phenomena. Everything is basically uncertain. The so-called laws of nature are only worthless guesses.

N. You do not seem to understand that there are degrees of uncertainty. That stones would not fall to the earth when you let go of them is extremely unlikely. I mean to say unlikely for the inhabitants of the earth. And this is what we are taking about I suppose. Or did you perhaps develop a special philosophy valid here in Hell or in Heaven?

H. Since I was considered free of sin, my rightful place is in Heaven but there all philosophy is forbidden. My short vacations in Hell offer me the only opportunity to develop a philosophy but time has been too short. It would also be a difficult task since everything here occurs simultaneously and not simultaneously. Our conversation must be about conditions on earth. For me it is very possible that stones do not fall, for instance when you do not see them.

N. Our views are too different for a fruitful conversation. You have driven scepticism to absurdity.

H. This is possible. I am not insistent. But I cannot change my convictions. It is too late for that. I want to take leave of you in a proper fashion and without ill will. My vacation is finished. (*H. bows and disappears into the dark backdrop.*)

D. (*sitting*) You two are too different for a really interesting conversation. But here comes St. Augustine. I have never seen him here before and he is such a holy person that I cannot stand his company. (*D disappears. In the conversation between N and A there is a slowly increasing irritation between the two partners.*)

N. Welcome Aurelius Augustinus. I look forward to discussing God's grace with you.

A. How do you know my name? I have come here to talk with a famous mathematician John von Neumann.

N. I am the one you are looking for.

A. I am here for the same reason as you. I have quarreled with God. For a long time I have suspected that he does not draw a clear line against the Pelagians, those godless scheming vipers that were banned by the church. When I uttered my misgivings I was banished from Heaven and arrived here. For the first time. You know of course the Pelagian doctrine that man can find grace and eternal life through his own deeds.

N. I went to a good, old-fashioned school and therefore I know the Pelagian theories very well. Pelagius was a British monk. During his life on earth he acquired many followers. The Semipelagians had a theory that lies between Pelagius and what you consider is the correct doctrine.

A. Are there Pelagians left on earth?

N. I fear they are many but the word Pelagian is no longer in use.

A. Ah, that breed of vipers! I fought them with the sharpest tools of logic and quotations from the Holy Writ and I won brilliant victories. I did not live in vain!

N. Maybe. Would it be impolite to remind you of the victories of the Pelagian doctrine on earth? Pope Urban II promised forgiveness of all sins for those who joined a crusade to liberate Jerusalem. Later forgiveness of sins could be bought for money. The riches of the church come from those who gave large sums for forgiveness of sins and a place in Heaven.

A. I know but still I did not live in vain.

N. Of course I am not a Christian but when I start thinking about the whole question I am inclined to believe that the most logical position is that of a Pelagian.

A. Your position hurts me but since you are well versed in logic it is easy for me to convince you that I am right. God rules over the fate of man before and after death. Who is going to Heaven or Hell is decided by HIM.

N. (*Starts getting more and more impatient and impolite to A.*) Perhaps. But you cannot convince me if we do not start by accepting some axioms. Without axioms every logical chain is just senseless gibberish. This is also what Wittgenstein thinks.

A. I hear that you are made of the right stuff. I suggest just one axiom: God is perfect and rules Heaven and Earth.

N. I accept that. God himself told me that.

A. Let me first make the revolting assumption that Pelagius is right that man can gain eternal life by his own doings. But God rules over the thoughts and ideas of man. If he left part of these activities to man, he would not be perfect. As Paulus says: for by obeying the law no man is righteous before God. What comes from the law is the knowledge of sin.

N. You cannot bring in the word of Paulus. You must keep to the axiom.

A. Sorry, that was an old habit. I start again. We must make our axiom more precise at one point: only God is perfect. Then it follows that man is not perfect and that nothing that he does is perfect. Hence he cannot gain eternal life by his own force.

N. I object to your logic. Man can do things that are perfect.

A. Not in my logic! Nothing is partly perfect.

N. Yes, but I cannot accept that you change our axiom. You added the word ‘only’. Please do not do that again. (*pause*) Let me change the subject a bit. How did sin come into the world? Do we not need an axiom about the law, hereditary sin and salvation?

A. No, and that is the advantage of my theory. God led man to his fall and the result was original sin. But God is perfect and hence he can do nothing without meaning. Of course I am referring to meaning in the sense of God, not that of man. His deeds are unfathomable but also perfect since God is perfect. God gives eternal life and a place in Heaven to some, but not to others. His name be honoured.

N. The honour was not part of the axiom.

A. But if we did not honour God he would not be perfect. Hence we must honour him.

N. We have not yet come to Jesus, the son of God.

A. Since God is perfect he has a son. Without a son he could not be perfect.

N. Should he not have a daughter, too?

A. (*angrily*) This I did not hear!

N. But death on the cross?

A. Through his son's sacrificial death on the cross God gave mankind the possibility of eternal life, a life that would have been Adam's without the fall.

N. Could not God have achieved this without sacrificing his son?

A. You talk like a miserable heretic. The ways of God cannot be fathomed.

N. Since God is perfect he must have created the Devil and all evil. Do you agree?

A. You talk as a heretic. I turn away from you with disgust.

N. But listen! The word perfect also means complete. God created everything did he not?

A. There is an abyss between God and evil. But I admit that what you say follows from our axiom. But remember that we are dealing with pure theory.

N. Do unborn children carry original sin? Must they be baptized in the womb or at conception to have the grace of God? Why should not conception itself be baptism? It is the work of God or is it not!?

A. Now you are getting insolent. You are worse than Pelagius himself. The church teaches that a child should be baptized within eight days. Otherwise it is eternally damned.

N. But how can you, a man, predict the ways of God? Eternity is God's realm.

A. That is no contradiction. God speaks through me.

N. Another axiom?

A. Do not be insolent.

N. Does man have a free will?

A. Of course. He can choose evil.

N. Does God want him the choose evil?

A. Of course not.

N. But there are men who have chosen evil. And this cannot happen without the will of God. Since God is omnipotent, nothing can happen outside his will.

A. God's omnipotence is fathomless.

N. It seems to me that you have constructed a God with exactly the same properties as Chance. Chance is unfathomable. Chance gives to one health and sickness to another. It gives happy lives to some and unhappy lives to others. Disasters happen by chance and also lightning from Heaven.

A. You speak as your reason permits you to. Chance is not holy and not perfect. Besides, your argument is old. Certain Pelagians wanted to replace God by Fate.

N. Chance is perfect. No one rules over chance. God could throw dice about admission to Heaven and no one would notice.

A. (*Ironically*) Perhaps you remember that our axiom says that only God is perfect. Hence Chance is not perfect.

N. You yourself added the word 'only' to our axiom. I never accepted that.

A. You may have a sharp mind but you are not a believer. I insist on the word 'only' in our axiom.

N. I am a believer in my own way. I believe, for instance, that you have chosen your axiom in order to counter other believers who think that God has properties that say something non-trivial about him. You say nothing that can be verified. In this way you are invulnerable but also empty. Your theory cannot be falsified. Hence it is empty.

A. You use words that I do not know. I understand the word falsify abstractly but how is it used?

N. To falsify means to prove that a statement is false.

A. What you say fits my experience. No one has proved me false.

N. That is because you have deprived your theory of God, grace, belief and doubt, every ounce of content. It can be accepted only by those who doubt their own intellectual capacities.

A. I am very learned and I have had a good standing through fifteen centuries. No one doubts my intellectual capacity.

N. I do, although my standing has lasted for just half a century.

A. This ought to make you cautious.

N. On the contrary. I am a seeker of truth. My human good sense says that the deeds of God cannot be separated from those of chance. Perhaps I should found a church for the adoration of Chance. This would be more honest than your pirouettes with the holy scriptures.

A. Blasphemer! Son of a viper!

N. God may send you to Hell for good. But one never knows. Maybe your stay in Heaven happened by chance. Or the opposite. No one knows.

A. I know one who never will leave Hell. You blasphemed and defiled God. But I did not.

N. (*Teasing*) You have told God that he is a Pelagian! God is a Pelagian!

A. Liar!

N. God is a Pelagian and you are an idiot!

A. (*Raging*) The only idiot around here is you, you son of bitch, God-defier, miserable heretic! (*A and N look threateningly to each other and start pushing* *each other and seem to start a fight. This takes a while but is disrupted by D. who runs onto the stage with a trident glowing at the ends.*).

D. (*Out of breath*). HE has seen and heard everything. He wants to strike you with thunder. You are going to court immediately. (*N and A are forced offstage by D with the trident*).

D. (*Deposes the trident that sputters in a can of water. Sits down, calms down and starts a thoughtful monologue.*) To-day has been a troubled day in Hell. It is very rare that HE acts so directly here. Most people are more cautious than this Neumann. His logic did not help him. On the contrary. (*Pause*). But what did he say? Didn't he say that HE is created by man, by the fright and yearning of humans? Just think of it! HE should be a phantom created by the imaginations of humans? How crazy can you get? This is absolutely ridiculous! ...But let me see now. What does it mean? That I would be created in the same way as HE. But of course not by yearning, only by the fright of humans. Their terror of torture and the ordeals of fire. This is a rather disagreeable thought. Something I do not really deserve...But there are consequences. If one wants to be logical. If HE and I and all the rest were phantoms created by human fear and yearning we can also be destroyed by humans. Suppose that the humans changed their minds or ceased to exist. That is a horrible thought. What then of us? No more eternal life, total destruction! No more Hell! Terrible! I must get rid of this thought! I shake it off! (*A short pause*) But it comes back. It is terrible. HE, I and everything here just phantoms that can go away any minute that the humans decide! No eternal life! No life at all! Total destruction! No,no this is just a nightmare! ...(*Rises*) It may only be a nightmare but I am starting to feel terrible. Terrible!. What if it is true? (*Leaves the stage, starting to cry and calling for help from God*) Help, help! HE must help me, HE must help me. Help, help...

Curtain

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GHOSTS I

3 Darwin Speaks Again

Late at night a modern biologist (B.) is sitting at his desk busy with his computer. Darwin (D.) enters suddenly, dressed in the manner of the eighteen-sixties, and a rambling conversation starts.

D. Please pardon my intruding. The reason for my somewhat abrupt appearance is that there are certain urgent questions that I should like to discuss with you.

B. (*surprised*) Yes, yes, very well, but who are you?

D. I'm Charles Darwin, the one who wrote *The Origin of Species*. I hope I am not forgotten?

B. No, no, not at all. But you cannot be Darwin. He is dead.

D. In my experience death is a relative notion when it comes to science. How I came here I do not know but now that I am here I have an opportunity to satisfy my main curiosity. I am curious to hear how the theory of evolution developed after my time. And I should like to talk with you about the principles of evolution. I hope that your are willing to do that and that you are able to disregard the somewhat odd circumstances that surround our meeting.

B. I will do my best. For a start, please take a seat. And may I offer you a glass of sherry?

D. No thank you, I am neither thirsty nor hungry.

B. Please don't think that the great Darwin is forgotten. *The Origin of Species* sells rather well after 150 years. It is a classic and readable, too.

D. Thanks for the compliment. It surprises me.

B. There is even an edition with all your changes and amendments done after the first edition. All ordered chronologically.

D. I worked a lot on my amendments but I do not think they are worth this kind of treatment. I understand from you that my work is the subject of exegesis like a fundamental religious document. I regret that because I did not found a religion. On the contrary, I only gave strong arguments that past life on earth developed by natural evolution which is still active.

B. I read recently that you borrowed some of these arguments from a certain Mr Wallace.

D. As soon as I got to know Wallace's work I arranged that his work and mine were printed in the same issue of the Proceedings of the Royal Society. I did it at once!

B. But they say there was a delay of several weeks!

D. For the printing yes. But not otherwise. I am a gentleman.

But let me come to my question. When I wrote the book I used the term Natural Selection. I argued that it exists as a mechanism but it does not predict the course of selection. Later I adopted Herbert Spencer's catchword '*The Survival of the Fittest*'. I thought then that it was a good summing up. But I do not any longer think that. Which species survive? The fittest ones of course. But how does one distinguish the fittest species from the others before they survive or die out? Also fitness is never constant. It is always fitness with respect to environment and the fitness of others and these conditions change all the time. If you try to predict a bit of the future from some observed fitness of a species you must take so many things in consideration that prediction becomes hopeless. If you try to think over what it means, Spencer's catchword disappears into thin air. It is an empty tautology! Likewise if applied to individuals! It pains me that my fame may be based on a tautology. What is your reaction?

B. I agree that fitness depends on too many things. Some sixty million years ago a small asteroid hit the earth and destroyed with one stroke the fitness of big reptiles and created or improved the fitness of small mammals.

D. This is news to me but it illustrates the difficulties I just mentioned.

B. The survival of the fittest is now not taken seriously by scientists. But I must say that your book has certain other weaknesses. It happens many times that the author takes Nature's wonderful ways, for instance all exquisite adaptations, as an argument for Natural Selection.

D. I am conscious of that! But when I wrote the book I often took a fresh breath in order to resist this temptation. I regret that I did not succeed completely. But remember that the Stability of Nature— I mean the existence and stability of species— is actually questioned by the theory of evolution. The stability is a only a delusion caused by the short span of human life.

B. I agree completely with this view, but may I remind you what is said in the first edition about the appearance of workers in societies of bees and ants. You claim that Natural Selection makes fertile parents regularly produce both sexless and fertile offspring. This kind of reasoning is, if you please, just another reference to Nature's intrinsic ability to produce useful things.

D. I have a faint memory of this passage but I wrote it long ago and may perhaps be excused for small lapses in my big project. There are more important things to talk about.

B. I see your book as a plea that life on earth could not have developed by means other than Natural Variation and Natural Selection. What you say here could perhaps have been more easily accepted if the Bible had had a slightly different account of Creation. The phrase *and God saw all that he made and it was good* could have been *but God saw that not all living creatures that he had made were good and he struck the bad ones with lightning and concealed them in the earth. And he made new creatures until he found everything good.*

D. But then it would be said that my theory is not new and I would have found it very difficult to get people interested in it. Fortunately the Bible says what it says.

B. In order to avoid every form of creation you assume that life has an intrinsic tendency to change. When this tendency has been active during a very long time, it has caused the appearance of new species from old ones. Evolution is like a tree with an insignificant beginning. Branch after branch appears, some die out, others develop new shoots.

D. That is not what I say. You are just replacing my long chain of arguments by a picture. But I admit that your picture is not entirely wrong. Note that I say nothing about the origin of life.

B. Well, let me have another go at your theory. Even though it can be criticized in detail no one else has a found a vision of life's development on earth that has the same convincing power.

D. I am pleased with that, but I think that my book is more than a vision. There are arguments. Please do not forget the chapter where I discuss and counter objections to my theory.

B. Of course I do not forget that. But please note my strong choice of words: convincing power.

D. I noted that. But please tell me about progress after my time.

B. Sure. In your time it was clear that acquired characteristics are not inherited but it was not clear how inherent characteristics are inherited.

D. Well, I knew something from my experiments with pigeons and there is an extensive experience of inheritance among men and from the breeding of animals.

B. Yes, but now we have new information. It comes from the interior of the living cell. There we find the inner inheritance mechanism of all life in the form of molecules that form chains and big complexes. Some hundred years ago such complexes were found and called chromosomes. We men have a certain number of them, women one more. When an egg is fertilized it gets half its chromosomes from the male and the other half from the female and then when the fetus grows, the chromosomes go into every cell of body. It is believed that they carry various genetic traits which control the formation of proteins in the growing body.

D. Only believed? Where are the details.

B. Much is known about the chromosomes of the much studied fruit fly, but for man, for instance, one does not know any details. But now, let me continue. After the chromosomes one has found similar and simpler molecules, called DNA for short. DNA is a long molecule which has the form a double helix which becomes a ladder with steps when unraveled. Each step consists of two molecules called a base pair. There are only four kinds of base pairs (two if you disregard the order between the molecules). If you represent each of them by a letter you can visualize DNA as a very long word consisting of only four letters. This word is unchanged when the cell divides into two because then the ladder is cut lengthwise into two parts, each having the ability to create or assemble a copy of the missing half. My description is a bit unorthodox but I hope it is clear.

D. I can understand the helix, the ladder, the splitting and the copying that gives new DNA for new cells but my understanding ends there.

B. But there is more to come. It is considered that DNA carries the blueprint for the growth and death of an individual. Your DNA reassembles mine as two individuals of the same species do but they are not identical. Your DNA suffices to identify you. And this is used by the police

D. By the police, indeed! There must be better reasons. How was all this discovered?

B. By a new microscope leading to a new form of biology, microbiology. There is also molecular biology. The various chemical substances and proteins can be seen if a mixture is soaked up in porous material. Then they produce different patterns. There are also other methods. I cannot give any details here.

D. All right, but what do these discoveries mean?

B. DNA is a very long molecule with thousands of base pairs but they can be grouped into something called genes. The sequence of all genes is called a genome. Every species on earth has its genome and is characterized by it. But the details vary between individuals.

D. You seem to give me only formalities. Every species on earth is characterized by many things, not only its genome. And there are always differences to be seen between individuals.

B. Sorry. The genome is a blueprint for the life of an individual from birth to death.

D. Like a seed of a plant, maybe?

B. I do not know whether you are ironical or not. The cells of your seed contain the DNA of the plant. DNA exists in every cell. The novelty of the genome is that we may manipulate it. Inject new genes and so on. There are many details here. But there are high hopes that serious illnesses are caused by defective genes and may be cured by selective killing.

D. Interesting. But I am a biologist, not a medical man.

B. But I am glad you are interested. There is more to be said about the genes. We say that they carry information for the life of an individual in the sense, for instance, that the initial growth, the successive formation of specialized protein, is regulated by the genes.

D. Any proof of that?

B. Sure, it is possible to replace the genes of a fertilized egg by the genes of another individual. This has been done with sheep and the result has been two genetically identical sheep.

D. That seems convincing. But how many sicknesses have so far been cured by this genetical engineering?

B. You found the same word that we used. Genetical engineering. But its results so far are meager. Perhaps there is such a cure in one or two cases. But there are high hopes and much ado about it in the press.

D. Let me go back to the genes. I ask myself if they carry inheritable traits. It was a lot of talk about such properties in my time. For instance for horses. How to see if a young horse is going to be good at the race track.

B. The grouping of the genome into genes has to be done by chemistry and trial and error. They carry inheritable traits but in a complicated way. The traits that we can see of observe through action correspond to only a fraction of the genes found in DNA.

Let me also say something that I perhaps should have said at the beginning. DNA explains Darwinism. Chance variations of DNA differentiates between individuals and makes for different capabilities of survival and regeneration.

D. But this is Darwinism! What you say is that each animal and plant carries its own intrinsic quality, visible in all parts and characteristic of its species, but with individual differences. Darwinism began with this elementary observation and concluded from the existence of fossils that nature has evolved by Natural Selection.

B. You seem to have difficulties with the genes. Due to the discovery of genes, your intuition is now replaced by the chemistry of proteins.

D. Thank you, with your permission I still keep some intuition. But let me accept your genes for the moment.

B. Do you also accept that DNA and the genes constitute a more concrete foundation of Darwinism than what was known before? I mean that DNA is a source of variation which together with other variations, like chance of survival and chance to have offspring, explains Natural Selection.

D. I accept this as an alternative but you must understand that I can only see this as a confirmation of my own way of thinking.

B. I repeat that we only need to remember that the genes are in all cells and are copied to new ones, . . .

D. (*interrupting*) We have been through all that!

B. Sorry.

D. Let us talk about evolution itself. Anything new there?

B. Well, the imperfections of the information process in the cells is the origin of the constant modification of living matter. When new forms appear, some have a better chance of survival than others and in this way...

D. This is just the survival of the fittest and not an explanation of the evolution.

B. But admit that what I say has the ring of truth.

D. Unfortunately. But how does one verify whether someone or something is fit for life? Except for very clear cases and short range predictions I think the answer must be a verification *posteriori* after many generations. If ever.

B. Please excuse me if I say that you knew nothing about the mechanism of inheritance and wrote very vaguely about variation. But we know this mechanism and see how its variation makes evolution possible. That DNA exists in all living matter supports the theory of evolution. It is true for all forms of life and explains why evolution proceeds very slowly and by degrees and through intermediate forms.

D. But that is what I said. Without your DNA. But does it explain the direction and adaptations of evolution?

B. DNA variation makes certain individuals better adapted to life than others.

D. There you go again. I have told you that the word ‘adaptation’ here means nothing. It just has a seductive ring to it. The same for the phrase ‘fit for life’. What I mean is that when one writes and thinks about evolution it is too easy to burden the terms used, even the term Natural Selection, with some purpose. For instance that the object of evolution is to make better adapted and more beautiful living things. This may be a natural inclination of the human mind but that is all there is to it.

B. I will provide you with an example. DNA gave to the swift its fast wings and broad beak to make it fit for life at high altitudes where it can chase insects undisturbed by other kinds of swallows. This would have been impossible for the swift without its specialized equipment. I mean that I can use the phrase ‘best fitted’ in an extremely convincing metaphorical sense.

D. If you change DNA to God in your example, you get an old-fashioned, edifying example of the Wisdom of the Creator. Natural theologians used the same kind of stories when they described how everything in nature is well adapted to its purpose.

B. I do not want to abstain from my inclination to a bit of loose thinking. But I admit that you may be right from a strict philosophical point of view. But biology is not only philosophy.

I want to say one thing more about DNA. It does not change abruptly. Its complicated construction makes large modifications extremely unlikely.

D. But this is also my argument. Natura non facit saltum.

B. This is only a simple quotation. The Latin does not make it better.

D. But the argument is very explicit in my book. Evolution has progressed through intermediary forms. I quote: ‘Natural Selection can act only by taking advantage of slight successive variations; she can never take a leap, but must advance by the shortest and slowest steps’.

B. You just guessed. DNA is an experimental fact.

D. I did not guess. Please do not be rude.

B. Sorry. But I insist that DNA is a program of the development of its bearer through life to death.

D. Everybody knows that inherited abilities are very important. More than that, maybe. But environment is also relevant. Now you are sitting over there overrating the importance of your DNA. An entire life program. No one with any experience of life can believe you. Someone falls off a horse and the life program is finished.

B. Sorry if I was not clear enough. I mean a life program which is not influenced by exterior circumstances. In certain cases one can see in DNA that a person carries the germ of an incurable disease which makes itself felt later in life.

D. And how is this possible?

B. As I said before it is possible to identify all kinds of protein, including the dangerous ones. May I remind you of the successful experiments that resulted in an exact copy of a sheep.

D. Doing that on a large scale one could make copies of human beings. To what purpose? What happens in the ensuing generations? We have always known the dangers of inbreeding.

B. Science must always advance.

D. But here backwards.

B. You ridicule respected, hardworking geneticists.

D. Sorry, geneticists?

B. After the laws of inheritance became known we got a science called genetics. Its practitioners worked to improve plants by crossing. Now they work with DNA in laboratories.

D. Crossing plants and animals is very old occupation. I have some experience myself. With pigeons. Moreover, I was a biologist working in the field. You talk about laboratories.

B. That is the direction the development has taken. Technical apparatus, powerful microscopes, electrical gadgets, still more powerful microscopes. And typewriters like mine here. It remembers and stores what I write and prints it on demand.

D. I can imagine all this but I do not like it. Are there no people who just think and write?

B. There are many, many of them and they work under orderly procedures. When I think that I have done something worth publishing, I prepare a manuscript and send it to a journal. There are hundreds to choose from. But only theoretically because every journal has anonymous reviewers who may accept or reject what I have done. Different journals have different standards and if I doubt the worth of my work I choose a journal where I am reasonably sure of acceptance. Since there are thousands of people like me who want to publish what they write, this means that people write too many scientific articles. Most of them are soon forgotten because what is written in them represents only a minute progress of science. No one is able to read everything and most of it leads to nothing. But, as you might have wished with your question, there are people think and write.

D. In my time science was an affair for a small number of gentlemen and I think that was much better. But let us leave all trivialities. I want to go back to my question about why the best adapted ones should survive. How is this in the light of your DNA. If there is some light.

B. No irony, please. I only tell you what I know.

D. Sorry.

B. Since the structure of DNA is known but not the exact way the genes rule the production of proteins it is perhaps best to take your slogan as a tautology. We can't foresee the effect of a small change of DNA. And if we could do that, we could not foresee a future environment. But in isolated cases like the following ones we could perhaps say something. A male pied flycatcher is attractive to females if its white forefront is clearly visible. You may imagine that there is a piece of DNA that is responsible for this white spot. If it changes to be more effective, all male pied fly catchers will in the end have bigger white spots on their foreheads.

D. Until they are white all over like pigeons.

B. I do not mean that. Some other development would take over.

D. Your example is the same as the one with swifts, only less poetical and less striking. But my conclusion is the same as yours. The effect of adaptation cannot be foreseen.

B. I admit that, but I am not ready to say farewell to my seductive explanations. By the way, they are very popular in biology nowadays. A biologist has written a book called the Selfish Gene. There he says that the gene has only one desire, to live on in as many generations as possible at the cost of others.

D. But the little molecule cannot possibly have desire in the ordinary meaning of this word.

B. You are too literally-minded. By gene the author means both the individual and the genetic information it carries.

D. I do not believe that this is true. A deer buck wants to breed only during a certain time of the year. The rest of the time it strives to stay alive. Every living being strives to live on. That is the dominating instinct. Breeding comes second and only during certain periods. I do not like this author. Not scientific. I suspect that we have here another attempt to explain evolution as a result of Nature's inborn Wisdom.

B. Perhaps but in this it has to be taken as rather advanced. The author is well known and his thesis has invaded the popular biological literature. But I think he wrote the book to tell what biologists think about evolution. For instance that it admits altruism. Relatives do not kill each other because they share the same genes.

D. But it may as well be the environment. Relatives know each other and often live together.

B. I am not responsible for every opinion that I am telling you about. In any case there is always a tendency to ascribe a kind of wisdom to evolution. I once wrote a popular article about the altruism of birds. But I understand that it would not be of interest my guest. When all is said it perhaps best not to attribute any intention or superstructure to evolution.

D. Chance rules. This is also my view in the book. Don't you agree?

B. That Chance is supreme is perhaps not putting it exactly right. Chance is limited by everything that it has previously achieved. If it has succeeded in forming a stable species, there is not much room for Chance. I believe that it then can only do a little mischief in the DNA.

D. This is what I always thought, though I never mentioned the word DNA of course. There is something repugnant about the thought that our finely tuned Nature is the work of Chance. But nevertheless this thought must be faced and evaluated. This is what I did in my book.

B. To return to the beginning of our talk I want to say that our descent from the apes and the catchword 'the survival of the fittest' both have disappeared from scene. They are not taken very seriously and do not arouse any hard feelings any more. You need not have a bad conscience.

D. Thank you, I am not troubled by this any longer. But I am still not satisfied by my analysis. It should be more complete but I do not know how.

B. There is perhaps some consolation in the fact that you have analysed history, the history of the development of life on earth. Historians have the same trouble as we have. Few things are absolutely certain, evidence is almost always missing, experiment is out of the question and so on. The solution for them has been to write books where some coherent philosophy is applied to the history of some period. There are some master pieces of this kind of writing. And this is for historians an accepted way of doing things. So, if you excuse me, I think that it may be said that you have written what amounts to a great historical treatise of evolution on earth. If you consider yourself as historian you may perhaps be more satisfied and free of your (and mine) unfulfilled desires of more satisfying explanations of evolution in all its enormous complexity.

D. I did not think of it this way. Biology is not only history. It is a natural science where logic and strict reasoning is required and some prediction, too. When I think back on my writing I think it had a meaning. I was dissatisfied with what had been written about evolution and I wanted the truth. The truth is that life in all its forms has come about during a very long time without any plan or any general principles that we can see. This conclusion may impress one as trivial and insignificant compared to the theories of creation. But it is true.

B. But think of all sharp observations and arguments behind this truth.

D. Yes, but the result…

B. The task was too big, too many unknown entities were involved. The only possibility is a vision. The biologist cannot experiment over long intervals…

D. I wrote a chapter about instinct. It began without any definition of this notion. But in spite of that I managed to say a lot about instinct. It was a bit vague but not meaningless I thought. I believe now that man has an urge or instinct to explain everything. It is indispensable in daily life. You have to explain a lot of things, why it is deadly to fall from a large height, why a bull may be dangerous, why one should not be in the way of a four-in-hand in a sharp trot and so on. There are innumerable indirect proofs that this instinct exists. It commands its owner to find connections and leave nothing unexplained.

B. I think that your vision of life on earth is a beautiful result of this instinct. Nothing to be ashamed of. You satisfied your urge and many have admired the result.

D. So far we must be satisfied with that. But now I feel that I am no longer able to keep my earthly shape together. Goodbye.

D's body pales away. B. leans forward over his desk, putting his head into his hands.

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GHOSTS II

4 Hypotheses. A Discussion with Henri Poincaré[3]

A room with a desk and a computer. M., who is a medical doctor and a bit of a philosopher sits at the computer writing a letter. Suddenly the screen changes and is lit up by a message in capital letters: PREPARE YOURSELF FOR AN IMPORTANT ENCOUNTER. M. hesitates for a moment not knowing what to do. Then there is a new message: TURN AROUND! M. turns around and sees a small man in a black suit twinkling under his pince-nez. A conversation starts.

M. Who are you ?

P. Henri Poincaré. I died in 1912, for the moment I'm back from the other side. I have an important question for you.

M. Thanks very much. But which Poincaré? There were two of them, as far as I remember.

P. The other one, my cousin Raymond, was a politician, I am Henri, a French mathematician known for important papers in mathematics and physics. My three books about science made me known also outside the scientific world. I died after laying the foundations of a new branch of mathematics called topology.

M. I remember having heard about you. But mathematics is far from me. I am a medical man.

P. I come to hear about the fate of the hypothesis in the natural sciences. In my book on science and hypothesis I stressed the importance of hypotheses in these fields. Science is not all discovery. Hypotheses are guides for research and thinking in general. Fruitful hypotheses are sometimes as important as definite results. After a long time of reflection I now think that hypotheses are somehow universally useful. I should like to discuss this with you.

M. There are hypotheses in medicine but we prefer facts. With hypotheses we would come close to alternative medicine.

P. Your are talking about things I do not know. Please explain yourself.

M. Scientific medicine stands in opposition to charlatans that are often popular with the press. They have named their own activity alternative medicine while we are said to practice school medicine.

[3] In his booklet *Science and hypothesis, (1912)* the great nineteenth century mathematician and physicist Henri Poincaré reviews the great advances made in the natural sciences in his century which saw the birth of the theories of energy, electricity, light and radiation. All of them were first born as hypotheses. He concludes that the popular view of science as a series of uncomplicated discoveries is wrong. Instead it is the well formulated hypothesis that drives science forward. The wake of science is strewn with discarded hypotheses.

P. In my time quacks were also popular with the press. This seems to be for ever unavoidable.

M. Sure.

P. But what do you have against hypotheses?

M. They do not belong in medicine. There are plenty of hypotheses that would kill patients if taken seriously.

P. I wrote about hypotheses in the natural sciences. If you do not accept hypotheses our encounter is finished.

M. Even if I hesitate to use hypotheses in medicine, I am interested. I am a bit of a philosopher, too. We could talk in general terms. Please take a seat and let us just talk quietly together.

P. and have some hypotheses. By the way, it seems that you share the common misconception that a picture says *everything*.

M. I don't. I just described our various pictures, not the difficulties about them.

P. Sorry. Are you finished?

M. Not yet. We have also new drugs. The antibiotics can put an end to very many infections. In your time many died by pulmonary and other infections. Not so now. People die later in life by heart attacks and the like. Or cancer. We now know a lot about cancer and we can cure some but not all by radiation. Our diagnoses are now much better than before. We just send a sample of a patient's blood or urine and even a bit of tissue to a laboratory that makes an analysis and finds out very precisely what the illness is. The doctor reads the laboratory report, writes his prescriptions and passes to the next patient.

P. From what you say the work of a doctor could be done by an automaton. Anybody can be a medical doctor it seems.

M. No irony please. When I mentioned the word 'fact' in the beginning of our conversation I thought of all the tools from the natural sciences that help us to make a diagnosis. I went through the most important of them. They really are facts.

P. I can agree with you but with some hesitation. It seems to me that your pictures and analysis are facts only in relation to the rest of medicine which, I believe, must be a bit of what it once was, full of hesitation and guesswork.

M. Of course these features remain. We have many patients with diffuse symptoms or symptoms which we do not understand.

P. But then you cannot do without hypotheses. Without them you would be helpless and unable to decide a course of action.

M. This happens sometimes. There are of course cases where we can do nothing. But I should like to paraphrase what Molière's wood-cutter says about fagots. I mean that there are hypotheses and hypotheses.

P. Yes, if you like. But you must mean something more specific.

M. I mean that the hypotheses in your book are too special since they are only taken from mathematics and physics and the book was written at a period when these sciences were very successful. For me the word hypothesis is too big. In ordinary medicine we just suppose and guess and muddle around. If one drug does not help, try another one and so on. I remember that you said in the beginning that the word hypothesis is used about causes and connections. I have very little of that, just standard rules.

P. I think you have explained yourself clearly. I may have been too insistent with my hypotheses. Perhaps I have been too optimistic when it comes to medicine. I agree with you that there are hypotheses and hypotheses. But let us continue anyway. You have told me many interesting things and our conversation amuses me.

M. As I told you we can now see that something physical happens in the brain of a patient when he is asked to think about something specific.

P. That is good enough but you have told the patient to think. Your experiment only says that thinking occurs in the brain.

M. You are right. Nevertheless we were happy about seeing what we may call a thought. We also saw another phenomenon, namely that thought precedes action. A simple example: when a patient bends a finger this action is seen first in the brain.

P. I had the same – of course entirely unscientific – experience many times. Before I write something on paper it has to be in my brain first. And before rising from my desk I had the impulse to do it. Unless I was very concentrated on something else. Then this movement was more automatic, if I remember right. Before making this kind of experiment I think one should try introspection first.

M. You are making fun of me. Nothing seems to impress you. But I try again. That actions start in the brain, can we not see this as an hypothesis?

P. I think not. It is somehow too obvious.

M. But let me take something from ordinary life: A man is going to cross a brook on a narrow footbridge. He hesitates a bit but then he thinks that this looks rather easy. This is his hypothesis. Then he falls into the brook and his hypothesis is contradicted. How about that?

P. I do not want to use the word hypothesis here. The situation is too trivial.

M. I read about you that you once had thought a lot about a mathematical problem. And then, as you left the bus in Caen, the solution passed through your head.

P. No explicit hypothesis was involved. Only a long period of preparatory work. That such things happen is not uncommon. A hypothesis must be the result of some serious thinking.

M. Our problem is that the word hypothesis is difficult to use in communication with patients. It is too vague and can be misinterpreted. Doctors, by the nature of their work, become bureaucrats in a way. And a bureaucracy cannot live with hypotheses.

P. May be I overrated the general usefulness of hypotheses. You are right that there are fagots and fagots. But in all kinds of serious research hypotheses are necessary. This is my last word.

M. But I still hope to satisfy you. Medicine is on the threshold of period of a very interesting research.

P. And what is that?

M. Fifty years ago it was discovered by X-ray spectroscopy that all living material contains long molecules having the form of double helices. They contain the secret of life.

P. What double helix? Explain yourself, please.

M. I do not know exactly how to describe it. The helix consists of two coupled spirals. If unwound the double helix takes the form of a ladder with steps. Each step has two parts with names that I have forgotten but the entire molecule is called DNA after chemical names that I have also forgotten. Each step has been given a name with two letters out of four fixed ones.

P. Hence there are sixteen ways of naming a step.

M. I believe you. You are a mathematician. But only four of them are used by nature and, if we disregard order, just two. If we give each step a letter DNA can be thought of as a very long word consisting of just four letters. These words differ systematically between species and a little between individuals of the same species.

P. I am amazed. Nature has a mathematical code.

M. Now comes the important part. Living matter consists of cells. When cells split into two, the DNA of the original cell halves itself into two simple spirals each of which is able to reconstruct the missing half from material available to it. Don't ask me how. The result is that DNA passes unchanged to new cells.

P. When Laplace worked with planetary movements he concluded that God is a mathematician. It seems that his hypothesis has now received an independent confirmation.

M. I am pleased to hear that you can joke a bit. By the way, does God exist on the other side?

P. May be. At least there are rumours. But let us return to your subject. A code is all right, but what is it supposed to be good for?

M. DNA is supposed to regulate the growth, life and death of protein in living matter.

P. So, DNA is the blueprint of life and death of all that lives. Is this the great hypothesis of biology and with it medicine?

M. Yes, or rather, was. Quite recently one has been able to read the DNA of man and divide it into tens of thousands of groups called genes which can be tied to well defined kinds of proteins.

P. How can you say that a catalogue verifies the great hypothesis? This is an illusion. One must also know the details of the action of DNA, not only a catalogue.

M. But there are genes tied to definite illnesses. It may be possible to cure them by some kind of genetic engineering.

P. My question remains. DNA is a wonderful code but you have to know in what sense it guides the birth, life and death of an individual. A multitude of questions come to mind. I believe that organic material can interact in enormously different ways.

M. There is hope of a solution, and a lot of money goes into molecular biology.

P. Only a very limited number of hypotheses seem to be essential to physics. But so far molecular biology seems to me not to be in the same situation. But my belief is that a limited number of well chosen hypotheses are always able to put some order into at least some parts of a recalcitrant material.

M. Maybe it is this belief that makes molecular biologists hopeful even when they have little to say.

P. Perhaps. But please remember that it is not possible to have too many hypotheses at the same time. That is too much for the human brain. We can drown in hypotheses.

M. You should perhaps address yourself to molecular biologists. Since my daily work does not stand hypotheses I have nothing to add. But what you say seems all right. We shall see.

P. Yes, I now have a got a lot to think about. It will be interesting to follow what happens even in the somewhat reduced way available to me over on the other side. I have now material for a second edition of my book, but unfortunately I cannot write it. I envy you your living conditions. Thanks and goodbye.

(*P. Becomes silent for a while. Then his shape dissolves and M. is left alone with his computer.*)

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THE SOUL OF SCIENCE I

5 Science and Common Sense

The characters of this dialogue are Simplicio[4] *(C.), representing common sense, and Lady Scientia, the guardian spirit of science. Their conversation takes place in a somewhere, entirely free of earthly appointments.*

C. I do not know how I came here or what I am supposed to do. You, dear Madam, may perhaps know something.

S. I do indeed. For a start we might perhaps introduce ourselves. My name is Scientia and I love, protect and represent science.

C. I am Simplicio. My friends think that I am the embodiment of Common Sense. I can say without bragging that I solved many a dispute with my common sense.

S. Do you happen to be the Simplicio who appears in Galilei's famous dialogues?

C. Yes, that's me.

S. I believe that I remember that Galilei, masked as Mr. Salvati, had great trouble convincing you that Aristotle's thesis that heavy bodies fall faster than light ones leads to contradictions. But is that right? Don't stones fall faster than leaves?

C. Do not test me, please. The reason for the different velocities is that stones and leaves have different air resistances. Galilei himself reduced the problem to heavy bodies of the same density and form.

S. Sorry, but how were you convinced? It is a long time since I read Galilei's book and my memory of it is a bit vague.

C. I was convinced in several steps. How it happened is a very interesting story.

S. Tell it to me, please!

C. Salvati convinced me by two thought experiments. First he assumed with Aristotle that the velocity of a falling body increases with the weight. Then he considered a small stone on top of a bigger one. At rest the small stone presses against the big stone. But this does not happen when they fall: if it

[4] Galileo Galilei was the first to formulate the law of free fall: air resistance being disregarded, all heavy bodies fall to the ground with constant acceleration. To explain this law, essentially the first example of so-called hard science, he wrote a collection of dialogues *Discourses and Demonstrations about Two New Sciences* (1638). The text argues against Aristotelian physics and the readers have to follow close reasoning and accept thought experiments. The task of one of the characters, Simplicio, is to put questions and receive answers which in the end convince him that Galilei is right.

did the smaller stone would increase the velocity of the bigger one and this does not happen. Hence a small stone does not fall faster than a big one. So far Aristotle may still be right.

S. And then?

C. Salvati suggested to put the big stone above the small one. If Aristotle were right, the small stone with its small velocity would then prevent the big stone from falling with its proper velocity. But together they are heavier than the heavy stone and hence, according to Aristotle, would fall faster than the big stone alone. It became clear to me that the view of Aristotle leads to contradictions. I gave up my trust in Aristotle but I also felt a bit sorry that he was not right. Later, when Galilei dropped a small and a large ball from the leaning tower and both hit the ground simultaneously, I was not surprised. I already knew that Aristotle was wrong.

S. Aristotelian thought was once considered to be common sense. You should not feel sorry that he was wrong. Common sense is a gift to man from birth and something to be proud of.

C. Of course I am proud of it. But Galilei made me change my view of common sense. It is open to improvement by thought and especially by thought experiments through which one discovers paradoxes that have to be eliminated. The result for me is that I now represent a modernized and developed Common Sense that does not dismiss thought and thought experiments. On the contrary. After my time with Galilei I did not find it difficult to accept Newton's rules of motion such as the inertia of matter: every body remains in its state of rest or uniform movement. If it is not subject to exterior forces of course.

S. What you say contradicts common sense. Uniform movement has only been observed during very short time intervals.

C. But this does not contradict common sense. I know as well as you, Madam, that most motions are not uniform when exterior forces are involved.

S. I was only trying to joke, I believe as you do that science has to work with simplified assumptions and thought experiments.

C. Otherwise there is no order. So says my common sense.

S. We could perhaps start discussing some interesting problems, now that we have so much in common. But first let us be precise and state the conditions of our discussion. Science always advances and therefore its position changes with time. I decide to adhere to the present position of science. And you, Mr. Simplicio?

C. Common sense is of course more constant than science, yet it, too, varies. Let me say that I stay by the present position of common sense.

S. But science and common sense have differed many times also since the time that the Catholic Church was its representative on earth. How did you, Mr. Simplicio, react to the rods of relativity theory which get shorter when they move fast and to the observation that time slows down in the same situation? It being understood that the rods could measure time.

C. I had of course great difficulty, but Galilei had prepared me. He taught me that there are many ways to understand reality and that numerical arguments have a purifying effect on all ideas that come from immediate observation. Therefore I came to see the theory of relativity (the special one to start with) as a model which put order into all the effects and properties that follow from the fact that the velocity of light in vacuum is independent of the velocity of the source. Let me also add that all these effects are too small to be immediately accessible to common sense.

S. You speak in a proper scientific manner, Mr. Simplicio. Bur how do you separate common sense and science?

C. I make a clear difference. Common sense does not create science. Its purpose is to observe science from the outside and at the same time understand it. Perhaps not all but the most essential and important parts.

S. But this means that I would be subordinate to your judgment, Mr. Simplicio. I must say that you have come a long way from the minor part you played in Galilei's dialogues.

C. Please do not do not excite yourself, dear Madam. Common sense is more or less shared by everybody. Just as you, dear Madam, is responsible for science, I am responsible for the right use of common sense in all weather. I believe that we could agree on the proper use and range of common sense. Without enmity and prestige and in all harmony.

S. I think that the picture that you paint is too idealistic, but I agree that we ought to be able to meet in civilized fashion as becomes decent people. But now, common sense has met worse ordeals than special relativity. I am thinking of general relativity and quantum mechanics. How did you fare with them?

C. The theory of general relativity raises more questions than it answers. For me it is a clever construction that can explain many phenomena that would be unexplained otherwise. If you excuse me I have found that this theory is not a fruitful ground for common sense. To me it is a beautiful mathematical construction whose value lies in the predictions that it makes.

S. It was nice to hear that at least some part of science remains free from the judgments of common sense. To me general relativity is the foundation of cosmology. Without it we can not say anything sensible about the universe.

C. You forget, dear Madam, that quantum mechanics is an indispensable part of cosmology.

S. Sorry about that, I went too fast. But before we continue it would be interesting to know how common sense reacted to quantum mechanics.

C. As I told you earlier, I learned from Galilei not to be afraid of abstract thinking. I accepted the foundations of quantum mechanics but I hesitated in the face of the difficulties that arise from the quantization of classical mechanics. But I think that a new generation of physicists have grown up with quantum mechanics are no longer worried by these problems. Certain parts of reality are now seen directly as quantum mechanical phenomena without a passage from classical mechanics. Permit me to say that this does not contradict common sense.

S. Look here, Simplicio, you talk like one who really knows what you are talking about. What you do not say is that your acquaintance with quantum theory is very superficial. You did not understand the mathematics of quantum mechanics and you did not yourself write a single article in the field. In spite of that you sound like a real expert. You got your views from reading popular reports. Such reports are only rarely written by people who understand what they are saying.

C. Madam! You are absolutely right of course! But please realize that if you force me to talk about science I must use the same phrases as the experts when they try to express things in a common sense language. But if you excuse me, my experience with Galilei has given me a general idea of what science is and I have found that this general idea is useful when trying to get some notion of more modern parts of science.

S. Please excuse my little explosion. It is clear that we sometimes use the same expressions from science and this obscures the fact that I have a deeper understanding of science than you ever can achieve. So when I say that the combination of quantum mechanics and general relativity has made possible a deeper understanding of the universe, in particular the theory of the Big Bang, I speak with some authority.

C. I agree that the Big Bang is a striking and audacious theory. But why the word Bang? No one heard this Bang and it is questionable that air was present to make it possible to hear.

S. Dear Simplicio, you must understand that the word Big Bang is a joke and that this joke has given the theory its name, not its content. Otherwise I agree with you that Big Bang is just a theory.

C. We should perhaps not bypass the new biology. I mean the discovery of the genetic code.

S. I find it amusing that Mendel's simple combinatorics should be followed by another one albeit not so simple. But I doubt the expectations that the genetic code alone is going to create order among all proteins and the way they are created and live in the human body.

C. Here you agree with common sense. We agree entirely.

S. This is not the first time that the range of a scientific discovery has been overestimated. I am thinking of what once was written about Newton's *Principia*.

C. Yes, I remember that. Many of these comments challenged common sense although Principia in itself was sufficiently sensational.

S. I want also to say something about the appearance of computers in science. The discovery and theory of semi-conductors was a very nice thing. The applications have meant a revolution in many fields, for instance all kinds of bookkeeping and numerical meteorology and other areas where theory can be subject to numerical computation. But those who talk about computers as a scientific progress do not realize what science is. It is really an activity...

C. (*breaks in*) You need not lecture me. Common sense can itself distinguish between science and what looks like science.

S. Excuse me, but this you cannot do without the assistance of science and, in many cases, time itself.

C. I am sorry that I overstepped my bounds. I hope you forgive me.

S. My dear Simplicio, I want to point out a serious, recent turn in the development of science which concerns both of us.

C. I am sorry that I do not know what you are referring to.

S. It is a phenomenon that I want to call the industrialization of science.

C. Please explain it to me.

S. In the last forty or even fifty years science in the sense of natural science has received more and more support from industry and the state. Both these donors, since they control the money, give rise to a new kind of scientist driven by a wish to be useful to state and industry and by the desire for money. Much of this is of course inevitable when the many applications of science are carried out. Perhaps science has been too successful for its own good. An outward sign is the fact that the number of scientists and scientific journals seem to have grown exponentially for some time. The journals that carry short accounts of scientific results and were once read for pleasure have grown out of proportion as have their prices. All this growth can be studied in the long catalogues free from quality control which are available to us by present information technology. All this makes my situation very difficult. An unlimited growth is not something that I or anybody else want to attend to. What once was called science has become a large market with all the signs of a market: a fight for money and the attention of the public. And attention itself attracts attention. There are trend analysts for science and the popularization of science. Earlier a scientific article used to have one author, now as a rule there are several of them. Scientific merit stands the risk of being collective.

C. I think it is only natural that science is industrialized because the world has been industrialized. Everything is now performed on a bigger scale than before. You used to admire scientists performing great feats of thinking in a simple world. This is a thing of the past.

S. My dear Simplicio now you are doing some phenomenological thinking. What you say is that things are as they are because of the way they are. But you are right that I do perhaps idealize the past. Please realize that quality in science is to me something that is almost independent of time. And I am a specialist in distinguishing quality. It is true that indifferent science has always been produced, at least after the eighteenth century. But now it is produced at fast rate.

C. Please give me some examples.

S. Earlier, biologists were peacefully studying animals and plants. Now after the first ecological scare they become ecologists and get new money for something they did not quite knew how to handle. But they write. And the scare that all oceans will rise to dangerous levels now keeps hordes of meteorologists busy.

C. Now that you have mentioned it, I realize I have noticed the same tendency. After reading the first page and the summary of a scientific paper, I often think that it is time to stop.

S. My dear Simplicio, you are now again masquerading as a scientist. Just reading is not enough to evaluate a paper. As an amateur you do not have the necessary insight to do it. I have said this before.

C. I admit my faults but Galilei and present company inspires me to express myself in kind.

S. Anyway, when I read scientific material, it takes a long time before I give up. My responsibility as a guardian spirit is clear. You used the word scientific not long ago. As a lover and guardian of science I must control everything that goes under that name. Recently this task has become heavier and heavier to me and also given me some unpleasant feelings. Simplicio! Science has definitely a soul visible to me in some of the best work done, and I believe that you can at least feel something of it. But now I can sometimes read entire volumes of scientific journals where nothing of interest seems to come out and the soul of science feels very, very distant. I have seen that the scientific method so beautifully applied by Galilei, is being applied nowadays to material that yields very little. And that some themes are being overplayed in the sense that only very small progress is achieved in every paper dealing with the theme. I do not quite know what to do, Simplicio!

C. Then, how should I know? The word science is perhaps not well defined. The definition lies in the user's mouth. The general public…

S. Let us leave the general public to itself. Otherwise we will never be able to end our exchange of views.

C. Long ago the situation was very simple. Science was an activity exclusive to academies and universities. But then there were no applications to speak of. Now applied science floods the market. This branch has a tendency to correct itself since its failures are costly or soon forgotten. One could say that it purifies itself. If you want some relief in your work you could perhaps leave applied science to me. I want to become the guardian spirit of applied science. It will be a suitable occupation for common sense.

S. A suitable occupation! You forget your historical mission! Common sense is free and independent from all and everything. As a guardian of applied science you tarnish your historical mission! What the world needs is common sense, not applied science. If you do not understand this, woe is to mankind.

C. I am sorry, you are right. I really regret my heretical ideas.

S. Now, when you said 'purifies itself' it made me think that science like all intellectual activity is subject to the same process. The next generation is always ready to criticise. Almost every established theory or belief is modified with time and some have a short life span. Science that is not fit for life dies on the shelves of libraries or in old hard disks. I feel I am getting some strength from this thought. I am now resolved to continue my work with everything called science, although part of my role is no longer that of a sweet guardian angel. I mean that I will read and evaluate everything as before but I will not always feel protective and nice. I will permit myself to hope that some things that I read will be forgotten as soon as possible. This feeling will make my life easier. It makes me optimistic for the future. And with better search machines for the net I could still fulfill my historical mission. I have made my decision and I feel relieved. My work is waiting. I thank you, dear Simplicio, for a fruitful conversation. Farewell.

C. It is risky to say farewell to common sense!

S. No cheap jokes please! Think of your reputation. Farewell!

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THE SOUL OF SCIENCE II

6 An Interview with Lady Scientia

An interview at the premises of the Royal Society, London, gives Lady Scientia (S.), the guardian spirit of science, an opportunity to state her views on science and what she sees as its soul. The reporter, Kay Cary (C.), is specialized in biology and medicine

C. When did you arrive in London?

S. I think we should switch to some important subject. Science for instance.

C. What is your opinion of British science?

S. We had better start with a definition of what science is.

C. Yes, please give me a definition.

S. Science is its own purpose and the purest expression of man's theoretical drive. Science means correct reasoning and methods and results not immediately accessible to common sense. My definition is not too precise but it serves to separate science from phenomenological knowledge. On the other hand it has to be specified to identify scientific elements of human activities like industry and agriculture and so on. But I believe that my definition can serve us for the moment.

C. What do you mean by 'the theoretical drive of man'? I never heard the expression before.

S. The drive to understand the world we live in by means of theoretical constructions.

C. Some words about phenomenological knowledge? Please!

S. Research that stays on the surface and avoids theory. Common sense is an example of phenomenological knowledge.

C. Thank you. Maybe I could represent common sense.

S. I have as much common sense as you. We have to share.

C. But common sense finds it often very difficult to understand science in all detail. That is a often experienced by a journalist.

S. You are right. I believe we shall understand each other. Let me first say that what we call science can exist only under certain conditions. Writing is a prerequisite and the scientist must have an independent position. These two conditions were first satisfied at the major royal courts of antiquity, for instance those in Babylonia and Assyria some three thousand years ago. The princes were of course more interested in their power and horoscopes than in science. But life close to the courts gave the scientists both leisure and independence.

C. When were you first interested in science?

S. Just about then. Three thousand years ago.

C. That is not possible.

S. But that is what it is. Possible. You must realize that I come from the other side. Now and then I assume a human shape and visit the world of humans. Nowadays I restrict myself mostly to academies. This interview, by the way, is a mistake by the administration. Normally I never meet the press. I am here to investigate the minds of certain interesting scientists but I have also other methods of finding out the truth. But now when things are as they are, let us continue.

C. (*Shows signs of uneasiness and panic but calms down after a while. Lady Scientia does not seem dangerous.*) Yes, well, let us do that.

S. First you must understand that, coming from the other side, I have no difficulty in reading scientific material. I make some excursions into the reality where you live in order to complete my impressions. Let me tell you a bit of my life as a guardian. My present life began when those in command gave me the task to guard science and investigate its conditions. That was about three thousand five hundred years ago. That my name is the Latin Scientia is no contradiction. It is simply a suitable name taken when Latin began to appear as a language of science.

C. Who gave you the task?

S. You ask too much.

C. Please excuse me. But I think that three thousand years cannot be enough. Were not the Egyptian kingdoms older than that and the Egyptian mysteries still more enigmatic than the Babylonian and Assyrian ones?

S. You have misunderstood me. I repeat that science means correct method and results not seen immediately by common sense. You must not, as does the public, confound religion and mysteries with science. These activities can sometimes use a kind of prescience but they have nothing to do with science. Perhaps one can say at most that Egyptian archaeology is a kind of science.

C. But the pyramids! Were they not built by science?

S. No, to draw a square in the sand and compute a slope is not science. Perhaps applied science and this is not my field.

C. Well, what shall we then speak about?

S. Continue the interview!

C. Give me an example of scientific achievement.

S. A Greek astronomer's giddying thought that the earth could be a ball that gets its light from another ball of fire, the sun.

C. Who was he?

S. The thought originated with an unknown astronomer and met with resistance but the arguments in favor became more and more convincing. This development fills me with delight.

C. Describe your delight to me, please!

S. Like everybody's delight. My feeling is personal. I want to keep it to myself.

C. Give me another example of science, please.

S. Euclidean geometry.

C. Why is this science? It is awfully old and taught in the schools to bored children.

S. Because the method of starting from axioms is spotless, because the results are interesting, because together they form a harmonious unity.

C. You forgot the bit about common sense.

S. Many geometrical results are intuitively true and therefore acceptable to common sense, but common sense uses only conviction, not arguments and proofs. Many results leave common sense cold, for instance that the axiom of parallels means that the sum of the angles of a triangle is half a turn.

C. This sounds terribly complicated. Do all scientific results have to be incomprehensible?

S. Much of it is now common knowledge, for instance that the earth is a ball. But the insight and the proof of this fact was science.

C. But all the philosophers, Plato, Socrates and all the others. Did they not write science?

S. They wrote philosophy. Philosophy requires neither strict logic nor results accessible to common sense. Philosophy for philosophers is one thing, philosophy for the general public has to be entertaining and offer some surprises.

C. Let me go back a bit to the royal courts. What about them?

S. I should perhaps make an exception for the ancient Greek republic. But Archimedes, for instance, lived close to the tyrant of Syracuse. The scientists of the old world had free contact with the political power; without this they could not have devoted themselves to free science.

C. I remember this Archimedes. Wasn't there something with a fixed point?

S. Yes, in a mythical statement. Archimedes wrote about astronomy, mechanics and large numbers. He proved that the area of the sphere is four times that of any of its great circles and other similar results.

C. Unknown to me. Can't we leave antiquity?

S. Not quite. The road-building and military art of the Romans was brilliant but not science. But when I think of the seventeenth century it is with considerable delight.

C. Why?

S. That was the heroic century of science. Galilei, Kepler, Newton, Leibniz.

C. Does their work really satisfy your criteria for science?

S. Almost all of it. Galilei's laws for falling bodies are logically perfect, not immediately accessible to common sense and verified by experiment. And then the great breakthrough: gravitation and mathematical analysis. You know of course that I am thinking of Newton and Leibniz.

C. Why do you always insist on the part about common sense?

S. Because I want to separate science from common sense.

C. And intimidate me and the greater part of humanity!

S. Try to understand some serious science and you will realize that common sense is not always a sufficient tool.

C. Maybe, I did not try much. In the seventeenth century you forgot Descartes and Pascal!

S. They would fit if we could disregard Descartes's philosophy and Pascal's religion.

C. You are too strict. Must your science always be perfect?

S. The word perfect does not exist in my vocabulary. All science is provisional and temporal.

C. And the scientists?

S. They are human and in general far from perfect. Newton made a serious study of the topography of Hell.

C. But relativity theory! Newton was wrong if I remember right.

S. I just said that science is provisional and temporal.

C. Excuse me! Could we not leave science for a while? Please describe again what you feel when you are delighted about something scientific.

S. You mean my feelings of delight in the seventeenth century.

C. Precisely!

S. I was of course not delighted throughout the entire century, only when I thought about the many important results brought about by the new possibilities opened up by the scientific method.

C. But isn't it an oxymoron that something as dry and involved as Newton's theory of motion and gravitation could cause delight?

S. You forget whom you are interviewing. My name is Scientia, I am the guardian angel of science, to use religious terminology.

C. I beg your pardon. But if we leave the seventeenth century, I come to think of Darwin and *The Origin of Species*. Any feelings about him?

S. Of course I know about him. My problem is to decide if what he did was science. There are many useful and necessary activities that are not science.

C. Yes, but really, Madam, I just happen to know that Darwin is our greatest scientist here in England.

S. I understand that I go against common usage of the word when I say that Darwin was not a scientist. He was first to arrive at the first sensible conclusion from the fact that there are remnants of many species on earth which are now extinct. From my point of view he represents am elevated form of common sense, since he arrived at an inescapable conclusion. I admit that my definition of science is not perfect. But that is what I go by. In my mind a large number of giants of erudition , for instance Linnaeus and all great historians share Darwin's position. It cannot be helped.

C. But dear Madam Scientia! I am shocked. All I learned comes to nothing.

S. Not to nothing, I stick to my definition of science and I ask you to respect it for the moment. By the way, now that we are in the eighteenth century, I must remark that the royal courts have been replaced by academies and universities as places for scientists. And in a new development the big foundations and the state have replaced the prince.

C. How?

S. They pay without interfering.

C. Oh yes!

S. In your 'Oh yes' I heard both irony and rudeness. Such things are not in order when you speak to me.

C. Sorry, I beg your pardon.

S. I cannot pass over my favorite century, the nineteenth century. Small universities, little money and good science that laid the foundations for all future progress.

C. Please give me an example!

S. For instance chemistry. I am thinking of the discovery of new elements and the construction of a list of all elements, valid in the entire universe and explained by the theory of atoms. It was the basis of the present chemical age with new materials everywhere. And physics: the discovery of electricity and the theory of electricity and magnetism which foresaw the existence of electromagnetic waves used in all global information systems.

C. Do you mean radio or television?

S. Both. It is the same theory. I do not have time to explain. For me it is something tremendous that humans by experiment and thinking have understood processes which are valid in the entire universe.

C. I have made a note of that.

S. We must try to have a friendly, respectful encounter. The present situation makes it impossible for me to explain complicated things in a few sentences.

C. I am sorry. Can't we leave the nineteenth century?

S. Very well. The first part of the twentieth century was just as good. From my point of view of course.

C. Why?

S. For instance Einstein's relativity theory and quantum mechanics.

C. Merciful God.

S. What do you mean?

C. It was a personal lament. You mentioned two things that are notoriously difficult to understand and explain and that go against common sense.

S. If you excuse me, they are no problem for me.

C. Please speak about everything that happened after the war with television and the atom bomb and so on.

S. What you speak about has its origin in the science of the preceding century and a bit into this one but is not in itself science.

C. It seems that nothing that I know or understand is science.

S. That's about right. And it isn't your fault.

C. Did science end after the war?

S. No, but the funny thing is that I don't have more to worry about now than earlier in spite of what is said to be accelerated progress.

C. How is this possible?

S. I do not know but it is so.

C. But when I think about the situation in the West, in the USA and England, where there are many new universities, discoveries arrive almost daily and there is an extensive press coverage of science. I think that this means more science.

S. I keep track of all important progress in science and the field has not increased qualitatively.

C. Can this be really true?

S. This depends on two things. Science is becoming indispensable in warfare and the results of science can be used to earn money.

C. Now you seem to have turned to a different subject, contemporary history. Not such a scientific a field, I assume.

S. You are right but as a historian I limit myself to science. I do not despise phenomenology and what is generally called science. As I said before both are indispensable in human culture but they are not science as I see it.

C. Cheers!

S. That was not entirely complimentary, I understand. To explain to you my present situation and that of science I must go back about fifty years.

C. I am waiting.

S. The prince has changed his relation to science. Everything depends on that.

C. But there are no princes in science any more.

S. I know well that the role of the prince as a prerequisite for science has been taken over by the national state, but remember that I have a long perspective. My prince is a metaphor for something whose existence is necessary for science. Everything becomes clearer if I call the national state a prince.

C. I see.

S. So, fifty years ago, just after the war, the prince realized that science had been very useful and even essential for a victory.

C. An example, please.

S. Electromagnetic theory made possible the radar equipment that conducted the bomber planes over enemy territory. Radar gave the one who first used it an advantage. Relativity and quantum mechanics showed that a large energy quantity was available in an isotope of uranium. This became the atom bomb.

C. Was there anything wrong with that?

S. The prince started organizing science to further his own purposes. In this way an ulterior motive foreign to it was imposed on science. In this way it lost its soul and was no longer science.

C. Not science! I recite your own definition: Science means correct methods and reasoning and results not immediately accessible to common sense.

S. Your forgot the first part: Science is its own purpose and the purest expression for man's theoretical drive. In the new situation science is a tool for the prince's lust for power.

C. But nuclear power?

S. An application of quantum mechanics and chemistry.

C. Well, yes.

S. The prince can act fast and sometimes in a wholesale fashion. When the Soviet Union shot a satellite from Siberia into space around the earth the prince of USA showered money over science and even the linguistics of Siberian languages got part of it.

C. Interesting. More examples?

S. The prince in one Scandinavian country has repeatedly reorganized existing universities and created new ones to further his dream: science for everybody.

C. And then science is not longer worthy of its name. I suppose.

S. Quite right. In other countries the prince has tried to make an industry out of science and in this he was helped by his country's strong industrial tradition. Perhaps I should not blame the prince for all this but he certainly is involved, whether by choice or necessity I am not able to say. This new development has meant a flood of material labeled scientific. My unlimited capacity to read, understand and evaluate a scientific text is not impaired by an increasing load, but I am more than sorry to see so many articles that represent smaller and smaller progress compared to articles published before. Besides you see an increasing number of names in the list of authors. This is happening at an increased rate in biology, for instance in your country's most prestigious journal. I am sure you know which one I mean. The same phenomenon can be seen in physics and even in mathematics. Science is becoming diluted and man's theoretical drive is being industrialized.

C. And your feeling of delight is also diluted I suppose. As a science reporter I have some insight in what you are talking about. If the prince wants to industrialize science he has willing helpers. To be a researcher is not a bad profession. Lots of free time, good working conditions and an interesting job.

S. You are right. But not all forces that make humans work give good results. A progressive devaluation of science is the last thing that I want.

C. Maybe you should call a press conference and make your thoughts public.

S. You forget that I am from the other side and that my press conference will end in absolute bedlam when the press realizes where I come from.

C. Sorry, I did not think of that. But how will the public know about your ideas about the industrialization of science? I think they are very interesting.

S. I always keep myself in the background. And I have time. Truth will always come to light.

C. I want to write an article from my notes and I expect this to be a rewarding and interesting job. It is very unusual material coming from the premises of the Royal Society.

S. Yes, yes, well, then we are done. Good bye. Please do not shake my hand, it will give you a spooky feeling. Good bye.

When she arrived at her newspaper, C. found all her notes reduced to blank paper. And from the recorder one could only hear a quiet rustle.

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THE SOUL OF SCIENCE III

7 Scientific

Two young people, Elisabeth (E.) and Peter (P.), students of medicine and sociology respectively, meet in a café and discuss the significance of their Ph.D. theses. E. has a romantic view of science and P. is more matter-of-fact. In the end P. introduces a broad definition of science: everything that employs the scientific method. But E. is not entirely convinced.

E. Hi, it has been some time. How are you these days?

P. Not so bad. I started writing a thesis.

E. About what?

P. Broadband in the Scottish Highlands.

E. But they do not have it yet.

P. My supervisor has got money to survey the need and use of the new information technology in sparsely populated areas. Half the money comes from a Scottish source, the other half from the European Union. This permits him to support two graduate students. I'm one of them.

E. But what are you going to do?

P. For a start I am sending questionnaires to all women in the highlands. The other graduate student is almost ready with his study of men's opinion of broadband technology. I shall investigate what women think of all the new services. — But look here, you were also going to write a thesis.

E. I'm doing it now. It is about a gene that could have something to do with the Alzheimer illness

P. It sounds exciting.

E. I am lying a bit. It is my supervisor who wants to find the gene although we do not know if it exists. But we have started with a genome analysis of a lot of cases. After that we shall work with rats. I have to become a specialist on a group of proteins which may be involved. The advisor tells me what to do.

P. Mine does not do that. I work by myself. First I shall describe a theoretical background. After that I deal with the answers to my questionnaire and make a comparison with the work of the other guy. I guess that I shall find that women are less interested in broadband technology than men, and I shall suggest remedies.

E. Do you have everything worked out already?

P. No, but I guess the result. Can you guess yours?

E. That we find a unique gene, which can be neutralized by simple medication. Then Alzheimer disappears from the world.

P. That sounds too god. Stop joking. Do you have something that can be called a vision?

E. My vision is that we shall perhaps succeed with the rats. After that my supervisor calls a press conference and says that we have made good progress.

P. How do you know that rats have the Alzheimer sickness?

E. When they can no longer find their way in a simple labyrinth.

P. But this can be due to other causes. In my field we specialize in finding causes.

E. We take the thing with the labyrinth as a definition. You have to start somewhere.

P. That does not sound so good.

E. But your thesis! It is just showing the obvious.

P. It is not at all obvious. We have an extensive theory.

E. Yes, I know, Durkheim and the other guys. Derrida also, I believe.

P. You do not understand the first thing about sociology.

E. Maybe. But let us not quarrel about our theses. Sometimes I ask myself if I am working in science or some industry. I could just be a small cog in a large machine.

P. Maybe you but not me. What people think about this and that is an eternal question. There are forever new circumstances. I am rather satisfied.

E. Satisfied with what?

P. I got a job that leads to a thesis and perhaps a future job.

E. Me too, but why not try some thinking of your own?

P. That is what I do all the time.

E. Do you think of yourself as a scientist? Somebody who has a big problem which is important for humanity and occupies his mind all the time?

P. I do not. But I am thinking of the problems that have to do with my thesis.

E. But do you think that it is important?

P. It is important to know how women see the new information technology. At least as important as preventing ten Alzheimers for a few months.

E. Now we are there again. Let us talk more generally. I believe that science these days is an industry and I feel that I am working in an industry. Please say something about this.

P. I'll be trying. My problem comes from some thinking committee in the European Union, not from me. But I am not part of an industry. Perhaps some service organization.

E. But that is a kind of industry. From where did the Union committee get its problem?

P. I suppose that somebody with a sense of the winds of politics found out that the Union must do something for sparsely populated areas. And the new information technology looked like a natural helper. And after that there was a policy meeting with few people and later a meeting with more people that made the decision. Many states have interests in broadband technology.

E. Very good. A perfect sociological analysis. And you are the obedient servant of the Union, on hand for every wish.

P. That has only a grain of truth in it. Whose obedient servant are you?

E. That is not so simple. Of course I am the servant of my supervisor. He leads our project and cannot work without servants as you say. But there is no one above him. He has chosen our problem, and put it on the Science Foundation market. There is no one above him I think. Perhaps he is the real scientist.

P. No, he is not independent. He is a prisoner of the gene racket. If he cannot find anything better there is always an illness and a gene. He is entirely in step with the times. Of course I can only guess. I know nothing about the field but I read the papers.

E. I think you are essentially right. The industry where I work is the gene racket. You gave it a name. On the other hand we are driven by noble motives: to cure and mitigate human suffering. But that is something one hardly ever thinks about in everyday life.

P. Do not take the word 'industry' too seriously. The discovery of DNA had to lead to an industry. Inevitably. The possibilities it opened up can only be realized on an industrial scale. Nothing remarkable about that. Sociologically speaking. And in an industry one is always like a cog. You must not have a romantic view of science.

E. Maybe I am a romantic. And this means that I think it is sad to be a cog. One does as one is told and this is the end of it. I mean a thesis.

P. But you are not only a cog. Think of ourself as a member of something bigger, a team. All the time you get to know what the others do and how everything hangs together.

E. I am still a revolutionary. I think that what I do is shabby. And you ought to think the same.

P. What I do is not shabby. It is important to know what women in sparsely populated areas think about broadband and the new information technology and how the could use it. It is important for the future of these areas.

E. Important for anything else?

P. For the Union and for everybody who sells the new technology.

E. Yes, maybe. But I'm not letting up. What we do, is it science?

P. Yes, because we use a scientific method. So it is science.

E. That makes science very comprehensive. So broad that it accepts any amount of indifferent material.

P. The word indifferent is personal. What is indifferent to one is important to another. Try to define science yourself if you can.

E. Your definition presupposes that we know what a scientific method is. You shift your definition of the concept of science to the concept of scientific method. How does one know that a method is scientific?

P. In what you said before you accepted my definition. You knew implicitly what scientific method is.

E. I admit that. But what I knew I knew from examples. Scientific method in a field is what is admitted by established people in the field. There is something of an official stamp on the word scientific.

P. I can't define the word better than you just did.

E. Good, now that we know what we are talking about we can continue.

P. How?

E. We could evaluate where we stand scientifically. You and I. I am sure that we are working on the lowest level of science. We are insignificant workers with very little knowledge of what happens higher up.

P. Speak for yourself. It may fit you but not me. I have my questionnaire and I am going to do some in-depth interviews myself. No one is over me.

E. There is someone. Your supervisor, Without him there is no Ph.D. He has to say that you are good enough.

P. I know he will.

E. No doubt... But you cannot say that what you do is great science. It started with somebody in the Union waking up the needs of sparsely populated areas. And he or she thought about the broadband racket and saw that it fitted into the political ambitions of his employer. And then he or somebody else was convinced that the matter was worth giving money to. What you do is science because you apply the scientific method to something that somebody else wants you to do. I do not claim to be better, although 'protein' perhaps sounds better to the public than 'sparsely populated areas'. Do you agree?

P. I agree with you but unlike you I like my work and think that it is important.

E. Please: I do not dislike my work. We are both in the beginning of something that could end as science. How many people do you think will read and quote your thesis?

P. I have not thought of that. Two, perhaps three, remarks in the proceedings of the Union and perhaps a line in a newspaper.

E. I think that is a realistic estimate. Science advances fast and everything done is soon obsolete. That a thesis is never quoted and lives only in lists of theses is a sign that it has contributed nothing except to the welfare of its author. I believe both of us have great expectations to end in this class. Like over seventy percent of those who write their theses with the aid of some grant and a supervisor. The sacrifice system of science. Our theses will end in the ashes of the sacrificial fire. I think that is a realistic prognostication.

P. You exaggerate. Your big mouth has taken command over you. Please do not mind that I say so. We have hardly started working and I do not yet feel the heat of the sacrificial fire. Anyway, they give us money. Shouldn't we pay and leave?

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THE PRINCE I

8 Archimedes[5] at the Palace

In his lifetime Archimedes was a friend of two rulers of Syracuse, Hieron and his son Gelon. In this dialogue Gelon (G.) has called Archimedes (A.) to the palace. Their conversation is an early example of the somewhat uneasy coexistence of science and political power that subsists to this day.

G. Welcome Archimedes. You were a dear friend of my father's. Now that he is dead, I invite you to form a friendship with me, his son.

A. I am much honored. But I am your friend already. We met many times when you were a youngster.

G. Please excuse my formality but as a new prince I feel that it is necessary.

A. Did you read my *Sand Reckoner*? I sent it to you last summer.

G. I tried but I lost interest rather early. Numbers were given to us by our fathers and I find no purpose in inventing new ones.

A. But my purpose was to show among other things that man can invent new numbers and compute with them. This is what our fathers did. And without large numbers and people who know how to use them for counting one cannot estimate the amount of food necessary to feed a large army. Of course Syracuse has no large army but for instance Xerxes had one. Without some counting and reckoning with large numbers, he could not have moved his enormous army from Persia to Greece.

G. As you said we do not need much of this here in Syracuse. Let me change the subject a little. During my journey to Athens I spent some time talking with philosophers on the Agora. It seems that you have a high reputation there. So now when somebody refers to Syracuse as a small place in Sicily I say that my palace needs a guard of five hundred men and that the fertile

[5] Archimedes (290 B.C. – 212 B.C.) lived the greater part of his life in the Greek settlement Syracuse in Sicily and is believed to have been killed when the Romans took the city. He is universally known for some long-lived myths: his mechanical feats in the defense of Syracuse and his proverbial *Eureka, Eureka!* when during a bath he realized that a body immersed in water loses the weight of the water displaced by the body. Actually Archimedes was the most innovative mathematician and mathematical physicist of antiquity. His many works written in Greek survived and have been printed. They served as a stepping stone for the seventeenth century inventors of mechanics and infinitesimal calculus. His only popular work is *The Sand Reckoner* where he estimates of the number of grains of sand necessary to to fill a ball centered at the earth and reaching to the sun. This was possible only by giving names to a body of sufficiently large numbers. In his preface he says that he is going to disprove the metaphor 'innumerable as the sands of the sea'.

soil of Syracuse has brought forth a mathematician and philosopher known all over the Greek world. But I wonder: how did you achieve such a wide reputation? Not from *The Sand Reckoner* I suppose.

A. I was always interested in astronomy and geometry and I learned from the philosophers in Alexandria. But I soon found out that I could do better than they. I constructed a machine imitating the movements of the earth around the sun and the moon around the earth. I found out that, contrary to common opinion, it is possible to measure the area of curved surfaces. For instance that the area of a ball is the same as the area of the rounded part of a circumscribed cylinder.

G. Surprising, but to what good?

A. No good at all except for the curious mind who wants to unveil the secrets of nature.

G. In the Athens *Agora* they told me that you have said: Give me a fixed point and I will move the earth. They accuse you of belittling Hercules and even Zeus.

A. I may have said something like that in some unguarded moment. I was thinking of the lever principle in theory, not in practice.

G. Please do not explain it to me. It must be for specialists.

A. The lever principle is applied a thousand times every day at the shipyard by uneducated people. Farmers use it to break new ground.

G. Yes, but without any terrible explanation.

A. You are right that most people do not think about the lever principle. Nevertheless I want to explain it to you. Take a long stick, support it at a fixed point close to one end. When you move the larger end it is easy to move a heavy object with the smaller end. Without the lever you might not be able to move the heavy object.

G. I understand roughly but without a practical demonstration I am lost.

A. Think of a farmer with a spit prying a stone from the earth.

G. I have seen that many times but I never thought of it as the lever principle.

A. I tried to describe the lever principle to you but you can only remember what you see and cannot turn my words into an abstract principle which is a thousand many times superior to an example because it embodies in itself myriads of examples.

G. Please do not try your moral principles on me. I am not a philosopher, only a tyrant. But let me now change the subject. You have revealed and want to reveal the secrets of nature. Can you also reveal the secrets of human nature?

A. What I discovered was only a small part of nature's principles. A multitude of secrets remain. Human nature is in a way known to everybody who lives a normal life of childhood, adolescence, adult life and old age. This means to have experienced maternal and paternal love, envy, human love, lust for power, feelings of humiliation and so on. Your expression ‘secrets of human nature’ is a misuse of the word ‘secrets’. I guess it comes from some soothsayer.

G. I believe some of the things they say. They reveal human nature to me.

A. With disastrous results, no doubt.

G. Please do not be rude. It does not become you,

A. And please do not treat me as a child.

G. I think that we do not quite understand each other because we lead different lives. What do you make of your life now that you have attained a mature age?

A. I think, I draw figures in the sand and, when this tires me, I walk around Syracuse and meditate on the lives of others.

G. Your life seems to me a very easy one with no duties except to yourself. My day is full of duties that you know very well. All the offerings to the gods, the trials, the executions, the festivals, the receptions, the palace guard and so on. And I must keep order in the palace, receive visitors and give and receive counsel. There is no end to my duties.

A. As you say I know some of them. But there is a difference between you and me. You can only partly enjoy my privilege: To decide for myself what to do.

G. I can if I want to. I am the boss of Syracuse.

A. If you say so, your highness.

G. I hear from your exaggerated politeness that you do not believe me. I am beginning to suspect that in your philosophical outlook on life only a philosopher’s life is worth living, not that of a prince.

A. I do not pass judgment about life’s worth. In our time princes seem to be absolutely necessary for other people to live normal lives. I mean that princes keep order in the society, chase criminals, deter people from crime by severe punishment and so on. Princes are beneficial to their subjects. At least this is a general rule with many exceptions. May I say that princes seem to be necessary to philosophers. Where there are philosophers there are also princes and cities. But the opposite is not true.

G. Ahh, my dear Archimedes. To follow your thoughts sometimes requires hard thinking. I realize that what you say about princes does not necessarily apply to me. Nevertheless I am pleased to play such important part in the society of men.

A. My measured general statement about princes does not contradict what you just said.

G. I am pleased to hear that. I may seem happy and powerful but do you realize that my life is in danger more than yours?

A. Of course. You have power and power is always under attack. There are personal enemies, palace intrigues and then the Romans.

G. The Romans are out to conquer the world. In their world there is no place for me. I do not see myself as a Roman satrap.

A. I can understand you. Have you made any preparations for a defense?

G. Yes but my soothsayers tell me that I will lead a happy life. Military things do not interest me much.

A. If the Romans attack will they come by land or sea?

G. I do not know. My advisers have no opinion in that matter. Except one. He says the Romans are building a fleet.

A. I find this interesting. I often go down to the shipyard to see the workings of the cranes and other machines used to move heavy things.

G. Can you help to build stronger fortifications? We shall perhaps need them. I can give you command over a thousand soldiers.

A. Maybe we need stronger fortifications. But I think I may also improve the old catapult at the shipyard. It is very primitive and has not been used for years.

G. Very well, I give you the task.

A. But if I do not accept it?

G. I am the prince. Nobody in Syracuse contradicts me.

A. Yes, your highness. I will do as you want but you must understand that I do not have the military skill to command a thousand men.

G. I believe your other skills are sufficient. You have a commanding presence.

A. But I am afraid that it is not good enough for a thousand soldiers. Soldiers are useless for what I am to do . I shall need carpenters, smiths and rope-makers.

G. I will give you what you want.

A. The Romans are not known for clemency. What do you think they will do if they take the city?

G. I am not a sufficient prize to be paraded on the Forum Romanum. I believe they will kill me and some uncouth Roman satrap will live in my beautiful palace. Since the Romans have no use for mathematics and philosophy they will kill you, too.

A. I fear you are right. We will both die. But in the meantime let me think about the catapult and other things in the harbor.

G. Very well. The audience is at an end because my duties await me. I wish both of us good luck. We shall need it.

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THE PRINCE II

9 A Dream

The relation of science to political power is further illustrated in a dream that the science reporter Kay Cary had after her meeting with Lady Scientia. It is recorded in the following dialogue between Ms. Cary (C.) and the prince (P.) who appears to her vaguely dressed in regalia.

P. I am the prince. Who are you?

C. I am Kay Cary and I am a journalist.

P. Then you are the one who talked to Lady Scientia! We two have common interests or rather some points of contention. To avoid an unnecessary discussion I inform you now that I am also from the other side and that I represent the experiences of political power through the ages. I am the essence of political power, if you please. You have to be courteous and respect me as a prince.

C. Of course.

P. I am sure that Scientia gave you a lesson about her favorite subject, the origin of science. According to her, the practitioners of science are always looking for a safe haven and free maintenance. They share these traits with other fortune hunters, soothsayers, artists, astrologers, inventors and historians, just to give you a few examples. What they all want they generally find close to the prince. This circumstance can be summed up very briefly: the attraction of power.

C. That is about what she said. I thought it very interesting to hear her description of the growth of science. Now I am interested to hear your opinion. I was amazed when she said the culture of Old Egypt did not have much science. What is your opinion?

P. It was not a sinecure to be Pharaoh. Too much to do with religion and one's own passing away and funeral and so on. For me it is not easy to say what is science and what is not. I talked to Scientia about the subject but unlike her I can only see the subject from the outside. I had a lot of builders and sculptors and hordes of priests. Some of them wrote history. So what do I know? My consuming interests were to conduct war and improve weapons.

C. Horrid!

F. And extend the might of my people!

C. Yes, Your Highness. But the Babylonians had science, didn't they.

F. The old kingdom or the new kingdom?

C. The new.

P. Not uninteresting. I visited some astronomers and saw their long calculations. But I was more amused by bards and soothsayers. My big interest was better arrows to be used against lions.

C. Lady Scientia admired Archimedes.

P. Yes, I hired him for some time. Mostly he went around thinking but he did not forget his meals. He was a bit of a bore but there was something about him. As a prince one must be able to judge people.

C. Did he not help in the defense of Syracuse?

P. Not much that I saw. I believe that most of it is mythical.

C. Am I really talking to Pharaoh and Babylonian kings? I am beginning to feel dizzy.

P. May I remind you what Scientia meant when talking about me. You must realize that you are speaking to an abstract concept, the notion of political power personified in me, the prince. Abstract concepts are very important in every discussion. To have concepts and use them separates man from animals.

C. (*confused*) Sure, it separates man from animals.

P. (*soothing*) That I am a concept need not concern us much now. Let us just continue. After all, you are a journalist.

C. (*recovers herself*) Yes, I am a journalist. Sorry about the interruption.

P. So, I continue. Warring is not all I do. As a prince I am responsible for the welfare of my people.

C. I have heard that before. In politics...

P. No irony, please! Remember, not once more!

C. I promise. In antiquity didn't the philosophers criticize the power of princes?

P. You are wrong. The philosophers depended on me and did not dare to criticize me very openly. They devoted themselves mostly to the human condition from an abstract and religious standpoint. That is why they can be understood long after they are dead.

C. How can you know this when war was such an absorbing occupation of yours?

P. I was not at war all the time. As young man I took part in some academies. Plato's for instance,

C. What did you learn?

P. I only got a general impression. No details. That is the way it is when a prince studies.

C. It must have been interesting for you to read Machiavelli's book *The Prince*.

P. I leafed through it but nothing was new to me. Others may find this book interesting but to us professionals it contained nothing new.

C. Listen to that!

P. Remember that I always mean what I say!

C. According to Mrs. Scentia real science started with Galilei.

P. I know her views. They are not mine. This Galilei had dealings with the Pope, not me. My scientific favorite from that time was Leonardo da Vinci. What drawings! I was very surprised to see how many things a corpse can contain. Once I wanted him to paint my entire court. But I hesitated. Scientists are risky company and I did not want to risk trouble with portraits that did not suit some of my beauties.

C. His picture *The Last Supper* became very famous.

P. Only afterwards. As I recall, the Pope was not pleased.

C. But now the seventeenth century. This Descartes.

P. A fine courtier and entertaining, too.

C. Isaac Newton.

P. There was much talk about him but I never understood why. That things fall I consider evident. Anyway, I had to care for him when he was famous. A simple pension was out of the question so I made him director of the Mint.

C. The great writers. Shakespeare.

P. Not at my court. I heard that these writers were discussed in my absence. But we must go on. Ask me something about the eighteenth century.

C. At about that time universities became important.

P. Maybe, but a very small post in my budget.

C. The French Encyclopedia became very important for science.

P. That book was a catastrophe for me. It incited the French revolution.

C. Do you still remember how it was to put your head under the guillotine?

P. Of course I do, but as an abstract concept one does not die so easily. Political power changes owners. For a time.

C. And how did that feel?

P. Natural. I remember that the conduct of wars changed. The Prussians started using breech-loaders. It led to a lot of shooting. Deafening.

C. War is not everything! What about the new way to travel?

P. I inaugurated many railways. The trains were shaky but they meant progress.

C. How about the rising tide of industrialism?

P. Surely I noticed. And the terrible anarchists.

C. But did you notice any science? I am trying to keep to our subject.

P. Science nested at the universities without troubling the prince. Except that I was given many honorary degrees. My religious duties were no longer so numerous and I could devote myself to my power and the welfare of my people. As Bismarck did at that time. — But look here, Ms. Cary, to get me to notice science, we have to pass to the Second World War.

C. Let us do that. What did you do?

P. I assumed so many different incarnations that it will take years to answer this question. Instead, let me be brief. Helped by this incomprehensible Einstein, another physicist discovered that some kind of uranium could split into two parts plus a lot of energy. This meant a super-weapon, born in a simple laboratory through quiet experimenting. Suddenly I had to revise my view of science. In all my incarnations. In one incarnation I got the weapon formula and wanted to keep it secret, as another one I wanted the formula and got it in spite of my adversary. The bomb became highest priority and scientists took part on all levels straight up in my own office. After the bomb was used twice, it became a scare that meant a lot of money spent for defense and new rockets. Perhaps I shall not burden you with all the details. As one incarnation I sent up a rocket circling around the earth and as another incarnation I answered by putting a man on the moon. In his place I now think that that was a costly mistake. I got nothing out of it expect paying through the nose to go to other places in the universe.

C. You sound rather cynical.

P. I am the prince.

C. Your life with science after the war. How was that?

P. Manifold. Several things became clear to me through my initiatives.

C. What initiatives?

P. I tried to have conferences for politicians and scientists. A complete failure. The two groups did not understand each other at all. I also realized that the scientists fight each other. But I had to pay more and more and create a foundation for science supposed to revise science periodically and to give grants. It is now so big and influential that the chairman is one of my incarnations. A prince of science.

C. How did you react to the two gifts of science, television and computers?

P. I took them as they came. Politics remains the same in our now democratic world. It meant that political power was divided and as a consequence there are new incarnations for me. Some interesting ones also.

C. A many-headed prince.

P. That is right.

C. Did you have some political advantage from science?

P. It adds to the prestige of the state and gives me something to praise and take credit for and brag about abroad. Indispensable for political power these days.

C. What is your most recent interest in science?

P. To fight it off. Scientists are very inventive, they always created new specialities and they always ask for more money. And they are masters of getting public opinion on their side.

C. Did you notice what Scientia calls the industrialization of science?

P. No. What is that?

C. The industrialization is the proliferation of scientific articles with a diminished scientific value. She suspects that too much material is written with the sole purpose of promotion. The fact that more and more names appear under the headings of scientific articles points in the same direction. As you know there is no promotion in science without publication.

P. That is not what my scientific adviser says to me. But it somehow fits with my impression although I did not put it in words. Ms. Cary! You just put an idea into my head. Industrialization and rationalization go together. I have a new weapon. A healthy reorganization is in order! Science has grown like an amoeba with no purpose! I will get my staff to invent and polish phrases like that and I will be able to reduce the scientific budget to a reasonable size! Public opinion and parliament will be with me! Ms Cary! Please excuse me, I have to leave you. Important work lies ahead. Farewell.

The prince fades away, ms. Cary wakes up and does not quite remember where she is.

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COMMUNICATION I

10 The Two Cultures

The fields of mathematics, physics and technology are considered useful to society but few students are attracted to them. The educator Frederick Forsyte with a formative background in political science and literature has seen the cause of this situation: the teaching of science does not employ the best methods available. His public campaign with this theme has attracted a lot of publicity but also some angry rejoinders.

In the dialogue below Frederick Forsyte (F.) confronts the teaching he criticizes. His science teacher for the occasion is Nomen Nescio (N.)

F. Welcome Mr. Nescio, I really want to know more about science, in particular what is called hard science, that attracts so few young students. I have a background in political science and a bit in literature and this may explain my curiosity. Let us start by using first names. I am Frederick.

N. I am Nomen. I feel a bit weighed down by my task but I will do my best. What shall we start with? Do you have a favourite theme?

F. Not really, only white spots. Maybe you could explain relativity theory to me.

N. Let me first explain the classical addition of velocities. Consider a person walking in the corridor of a fast train and assume that he is walking in the direction of the train. Suppose that his velocity is five kilometers an hour and that the train has the velocity of 140 kilometers an hour. In this situation an observer on the ground will observe that the person in the train moves with the velocity 145 kilometers an hour in the direction of the train. On the contrary, if the person was walking in the opposite...

F. But how can the observer on the ground really see the person in the corridor and much less observe his speed? Everything goes so fast that he has no time to think and no time at all to measure the velocity.

N. You are right, it was a stupid thought experiment. Maybe we could instead think of a person walking on a moving band in an airport. Then the observed velocity is his own velocity added to or subtracted from that of the band.

F. Added. You must mean increases and decreases.

N. Added means that if one of the velocities is a meters per second and the other b, also meters per second, then the total velocity relative to the ground is $a + b$ meters per second.

F. Formulas do not go with me. Please take figures instead!

N. If the band moves with 2 meters per second and the walker moves with the same velocity with the band, the velocity of the walker, viewed from the ground, or the floor in this case, is 4 meters per second. But if he walks against the band he does not seem to move at all.

F. Thanks. That is pretty clear. And now to relativity theory.

N. We have a long way to go.

F. But I have patience. What is the next step?

N. One hundred and fifty years ago, the physicist Fizeau found a method of measuring the velocity of light in air and water and other material. In vacuum, that is when air has been pumped away, he found the enormous velocity of 300 000 kilometers per second. The velocity is less in air and still less in water and more opaque materials. By the way, these facts explain the everyday noticeable refraction of light. But when Fizeau measured the velocity of light in running water he found the same velocity with or against the flow of water. Others after him made the same and better experiments and the result can be summed up very simply: the velocity of light is independent of that of the source.

F. How?

N. If you walk around with a flashlight in outer space and you light up an observer who can measure the velocity of your light when it arrives to him, he will always get the same figure whether you walk towards him or away from him.

F. I do not see the point of this. I never walk in outer space with a flashlight.

N. You must accept thought experiments. Without them one can't understand physics. Without thought experiments science runs dry.

F. Not my science. In my world only facts can be accepted. And I understand that also physics deals with facts in the form of real world experiments.

N. If I started telling you the details of the experiments whose conclusion is illustrated by the flashlight in outer space you would immediately start protesting. Too many facts and details.

F. I believe you.

N. I try again, also in outer space. Imagine that you are shooting pebbles from a slingshot towards an observer and that the observer can measure the velocity of the arriving pebbles. Then he would be able to notice if you moved towards him or away from him when shooting. If, for instance, you shoot standing on a rocket which moves towards the observer with a velocity of a thousand kilometers and hour, he should take care. And if the rocket went away from him, he would never see the pebbles.

F. Yes, clearly. But I find your thought experiment a bit drastic.

N. I have in mind a comparison of the pebbles and the slingshot with light and the flashlight. The results of the two experiments are entirely different. The observer finds that light always arrives with the same velocity while the pebble sometimes arrives with a large velocity and some times not at all. You must understand that the experiment with the flashlight made an entire world collapse.

F. What world? How could a thought experiment have this effect?

N. The world of commonplace observations and scientific thought about moving bodies. In our conversation the thought experiment must serve as a real one. We must be able to make hypotheses and pretend. To use make believe. Otherwise we shall get nowhere in physics.

F. Funny. In sociology make-believe is not permitted. One must have facts and theory. It is best to have both.

N. Theory is a form of make-believe, also in humanities and the social sciences.

F. That is not what we think. Theory is something that keeps together a large collection of facts.

N. But more often than not in a comprehensive and diffuse way, if you do not mind. In your fields of science, theory is mostly about interpretation. And do you not agree that theories in the humanities and the social sciences are often personal and rather imprecise? Like it is for philosophy, but good enough in spite of that.

F. Now you are talking like a wise, old humanist. But what you say is true only of certain theories. Others are very exact.

N. In physics and chemistry theory is something that has to make good numerical predictions. Within measuring error, of course. But theory is more than that. Theory is a tool for evaluating old and new observations and for thinking about coming ones. Theory is more than a summary of facts. A good theory of a phenomenon gives one a deeper insight into its nature, not only a description.

F. You are very eloquent. I can agree.

N. We could perhaps go back to relativity theory. It says that no velocity is greater than that of light in vacuum. As I said the theory started with the observation that the velocity of light is independent of the velocity of the light source. It shook am entire world.

F. What world? I asked that before but got only a vague answer.

N. Classical Newtonian mechanics. It is based on the addition of velocities.

F. Suppose, for completeness, that you give me a picture of Newtonian mechanics.

N. A picture cannot do justice to this theory. I have to start from the beginning.

F. Is that really necessary?

N. I will try to make it as simple as possible. Newton stated three laws of motion. The first one is that a body in motion, which is not subject to outer forces, moves in a straight line and with constant velocity.

F. An example, please.

N. You throw a stone.

F. It falls to the ground.

N. That depends on gravity, an outer force coming from the earth that acts on the stone. Gravity exists as a force between all matter. The more matter there is and the nearer one is, the greater force from gravity. On the surface of the sun you would not be able to stand and also burn but that is another story.

F. Your thought experiments are getting worse and worse.

N. I go back to the stone on earth. If you had thrown it in outer space at a place where the attraction from the heavenly bodies is very small you would have seen the stone move along a straight line with constant velocity.

F. But I have had enough of your thought experiments in outer space. Please stay here on earth.

N. OK. For a short time after the stone left your hand, it moved very closely to a straight line and with almost constant velocity. The effect of gravity can not be observed by the naked eye. But if you shoot against a goal with a gun you have to believe Newton. Otherwise you could not aim and hit.

F. To me Newton's law is wrong. It is true only approximatively and then only for a second. What kind of law of nature is that?

N. But you must understand that Newton's laws of motion express the inner core of his theory. All outer circumstances are peeled away.

F. But these are very important and cannot be avoided.

N. Newton's laws constitute the philosophical foundation of a theory of motion and they are verified by their predictions of planetary motion, weightlessness in satellites and millions of successful constructions of moving parts in machines.

F. That is all very good but I want you to explain Newton's *theory* to me.

N. Newton's second law says that the rate of change of momentum with time is proportional to the acting force. The third law, finally, says that to every force there is a counterforce, equal in magnitude and with an opposite direction.

F. This is impossible to understand. I hardly heard the word momentum before.

N. The momentum of a stone is the product of its mass and velocity, direction included.

F. How could you use the word without explaining it first? You do not follow current pedagogical principles. Can't you explain so that I understand?

N. To understand one must first have an example. I give you another one and regret that it takes place in outer space. Imagine a rocket with a weak but long-lived driving engine. By Newton's second law of motion it will with time increase its velocity to many times the velocity of light. But this contradicts the law that no velocity is larger than that of light in a vacuum.

F. But light and the rocket are entirely different.

N. Both are influenced by gravity. One of the first verifications of Einstein's theory was that light rays are bent by gravity when passing a big chunk of matter. The planet Venus, I believe.

F. Could we not leave light aside and occupy ourselves with Newton's theory.

N. To be able to really understand it you must first understand quite a bit of infinitesimal calculus and then yourself predict by computation a number of typical cases about things thrown and trains and cars colliding. After a while you would be able to deduce planetary motion as an exercise. How the planets move in elliptical orbits around the sun.

F. But I told you that I and mathematics do not go together. There must be a simpler way.

N. An encyclopedia addresses the public. There you can read among other things the following text about Newton's law of gravitation: '... a statement that any particle of matter in the universe attracts any other with a force varying directly as the product of the masses and inversely as the square of the distance between them. In symbols, the magnitude of the attractive force F is equal to G, the gravitational constant, a number, the size of which depends on the system of units... '

F. You told me this already in a simpler way and without formulas. I want better explanations that I can understand.

N. I did my best. I sketched a course of study. The only thing missing is a list of books you have to read.

F. But I told you that I cannot stand mathematics. And I share this predilection with 99 percent of the educated public.

N. This means that your wish cannot be fulfilled.

F. Maybe, but I am still convinced that I am right about simpler explanations. Moreover, if I remember right you said that there is something with light that says that Newton is wrong. And then I do not have to understand Newton. Besides, since his theory is wrong, it may be impossible to understand. Why is it not scrapped? I read that the ideas of Aristotle are all in the dust bin.

N. The velocity of light is immense, a hundred thousand times the respectable velocity of 300 kilometers an hour. Newton's theory is very good and for practical purposes exact for velocities that are much smaller than that of light. It is also interesting in itself and has any number of practical applications. There is no reason for you not to understand it.

F. I give up. Can't we start with relativity again?

N. It will be worse for you than Newton's theory. Classical mechanics fits very well with man's experiences with lifting and throwing. But relativity theory has no such basis in everyday life. We have no experience of extreme velocities. Finally, the mathematics that you shall need is much more advanced than for Newton's theory.

F. If what you say is true, I do not stand a chance of understanding relativity theory.

N. Now I will try a more phenomenological road. The theory says that time slows down as the velocity increases. For instance, if you embarked on a train that went around in a loop with almost the velocity of light and then came back, and we met again, I would be very old, maybe even dead, and you would look the way you are now. More: if you had been able to measure the length of a wagon on the train at the same time that I did it from the ground, your length would be much shorter.

F. You are giving me fairy-tales! Your thought experiments are getting out of hand.

N. Sorry.

F. What is it in science that makes it so hard to understand?

N. I believe that the difficulties are mostly in the exact sciences and mathematics. They are there because everyday experiences of man do not suffice as a background or paradigm for the mind. Perhaps the necessary paradigm has to be hammered in first. After that it is possible to understand.

F. I detest the word hammered in. You seem to prefer old-time teaching. As you know it is fought by the entire school leadership.

N. I mean that the study of the subjects in question requires both time and a kind of inner absorption. When the school also has to produce results with less willing pupils only a bit of rough teaching will do. That most of the stuff disappears from their heads after some time when not used is only natural.

F. I think you are wrong. There must be a way. Everybody has the same kind of brain.

N. That is true. But I repeat: everyday experience is not enough. It suffices for many things like political science and general statements about animals and vegetation but not for the exact sciences physics and chemistry. And not at all for mathematics.

F. You are wrong. Political science and sociology have many theories and most of them are difficult to understand.

N. You can say that with a certain authority. But I think that the source of the difficulties lies only in an extended terminology. The basic facts are generally accessible to the educated public. It shares its basic experiences of society and daily life with the originators of all these theories.

F. You are wrong. There are theories of state and democracy that are very difficult to understand even for me. There is a great gap between the naive reader and advanced political science.

N. Let me take Derrida or some other willful sociologist as an example. It may be difficult to understand what he means but what he says is more often than not personal interpretations based in some abstruse intellectual tradition. In science we have constructions and notions that are supposed to be understood by anybody independently of cultural background.

F. Not everybody. You have to make an exception for me.

N. I meant everybody with enough time, interest and motivation to understand.

F. Thanks for the compliment.

N. Let us continue without personal remarks.

F. I agree.

N. If you excuse me, I have a theory about why you wish that scientists should explain their theories better to students and the public. You are led by your own experience that the social sciences and literature can be explained to the public even when originally presented with an overdose of terminology.

F. That is not my opinion.

N. Let me take the press as an example. When the press wants to explain cultural matters to its readers, the material comes from the social sciences and the humanities. My explanation is that this material can be explained to educated readers and also has an element of entertainment in it. Otherwise it could not motivate its existence in the press.

F. But the sciences, too, are written about in the press.

N. But only when the material satisfies my criterion of being understandable by educated readers. The nuclear bomb provides the background to physics, new materials to chemistry. Theory has no place.

F. But it is not right to take the press as an example. It has been watered down more and more to satisfy a decreasing ability by the readers to accept serious material.

N. The watering down has had an effect on the frequency of cultural material, not on its quality.

F. Yes, I believe you are right. I believe also that my lesson should end here with a confession. In order to survive in my bureaucratic profession I must now and then take some initiative especially when journalists are present. Therefore I once said that scientists ought to explain their results better to the public and in the schools. I think the same now but I have no illusions of being taken seriously. Most people who heard or read my message probably saw it as a pious hope if they even noticed it. That you took it seriously can perhaps be seen as professional mishap. Yours and mine.

N. After this ambiguous statement I give up my pedagogical efforts. But I hope that our conversation has disturbed a certain smugness. Whose it is I do not say. Goodbye.

F. Goodbye.

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COMMUNICATION II

11 Metaphors[6]

Below, a somewhat aggressive journalist (J.) is interviewing Boriander (B.), professor of physics, in his office.

J. You have just published a book about the inner secrets of atoms. Is it possible to explain what this book says?

B. No one knows the inner secrets of atoms. My book is only a review of the difficulties one encounters when trying to combine gravity with electromagnetism and nuclear forces. Whether these difficulties can be explained or not depends on the reader or listener.

J. But the book has received a big prize!

B. Naturally, I am happy about that!

J. The public always wants to hear more about science. Couldn't you try?

B. I don't think it is a good idea to shower the public with technical language.

J. As a member of the general public, I agree completely with you. But I think that I and my readers could need a short introduction to your kind of physics.

B. Sure. Every chemical element consists of only one kind of atom.

J. Element?

B. For instance boron and cadmium.

J. They are unknown to the public. Are there not simpler examples?

B. We can take oxygen and hydrogen. We breathe oxygen and there is hydrogen in water. Water is a chemical compound of oxygen and hydrogen.

J. Couldn't we simplify a bit and take water instead of hydrogen. Everyone knows what water is.

B. But water is not an element. As I told you it is a chemical compound of oxygen and hydrogen.

J. Sorry.

B. I repeat: every element consists of only one kind of atom. Every atom consists of a nucleus and a shell of electrons.

J. How shall I think about the nucleus? As a stone in a plum?

B. It is too concrete. Just think of it as something heavy in the center of the atom.

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[6] X-rays, a Nobel prize, relativity theory and the nuclear bomb made physics a subject for the media. To convey a sense of the theoretical side of physics to the public, metaphors are a necessity.

J. Such as a stone in a plum!

B. This metaphor is too concrete!

J. All right, but this shell of electrons?

B. An electron is a very, very small particle carrying a negative electric charge.

J. But shell?

B. The word particle cannot be taken at face value. We could say that every electron turns around in an orbit around the nucleus. It is this orbit that constitutes a shell. Many electrons give many orbits that together constitute a many-layered shell.

J. Can I say that the electron turns around so fast that it can't be seen?

B. Unfortunately this is a meaningless statement. We cannot see a single electron, only its action as an electric charge. That it turns around the kernel is just a picture.

J. Shall we not go directly to the nucleus?

B. But perhaps first to the periodic table.

J. And what is that?

B. The elements can be ordered according to what is called their numbers. The number of an atom is the number of electrons it contains in electric equilibrium. The numbers of the elements go from 1 for hydrogen to around 200 for and lead and uranium.

J. This tells me nothing. Why the word periodic?

B. One can order the elements in periods with similar chemical properties.

J. What you say is getting meaningless to me.

B. It was perhaps not so smart to start with the periodic table. It is all important in chemistry but maybe not just now. So I start again. Every nucleus is built in a complicated way by gluons and quarks. The Greek word *gloios* means a sticky fluid.

J. How does it all look together? Like plums in a sauce? I am sure that you realize what dessert I am talking about.

B. Maybe you are thinking of the quarks and the gluons. This picture is too sharp. The quarks and gluons can't be seen. There are also larger units, positrons and neutrons. Your metaphor is both useless and wrong.

J. I beg your pardon.

B. You must think in a more abstract way. Metaphors do not help.

J. But metaphors help my readers. The people that I write for. What I write does not make sense without metaphors.

B. Your metaphors are harmful. The right thing to do is to imagine the nucleus as something very small that consists in a vague way of quarks and gluons.

J. I love metaphors. Couldn't I say that the nucleus is like a piece of raisin cake? I mean with the quarks and gluons.

B. No. Your desserts do not give a good idea of the nucleus and its complicated structure. Just think of the nucleus as very small and do not forget the electron shell.

J. That'll be very difficult. Perhaps a bundle of threads with the ends sticking out?

B. It is better but not needed. The atom is like a small peppercorn swarmed by very small flies.

J. Excellent! Thank you!

B. I did not mean that. I take it back. The atom is something very small consisting of quarks and gluons. That is all.

J. You forgot the shell!

B. Sorry.

J. But I try again. The atom is like a ball of white almond icing stuffed with small chocolate pieces and surrounded by curling silk paper. I think that is fine.

B. No, no please, no. If you write that you will scandalize me.

J. But without metaphors my evil chief editor will sack me.

B. That cannot be helped.

J. You are extremely heartless.

B. I understand your position but you must also understand mine. One cannot see an atom. It is only through theoretical physics and mathematics that we can say anything about them.

J. But that is not true. We can think that we see them. Atoms are small, small particles. All matter consists of atoms. The word 'small particle' is also a metaphor.

B. You are right. But if 'small particle' is all we knew about atoms and molecules we would not know more about matter than the old Greeks.

J. But they knew a lot, I think. Didn't they have atoms?

B. Perhaps. But they did not have the periodic table system, for instance.

J. And what is that?

B. I tried to start an explanation a moment ago.

J. Sorry, but I am trying to make an interview.

B. It is perhaps best that we start again with my book. It shows that the comprehensive theory, called 'theory of everything', which is is supposed to unite electromagnetism, the nuclear forces and gravitation, is logically impossible.

J. Gravitation?

B. That means attraction by masses.

J. Thank-you. What you say sounds very interesting. Theory of everything. But there is already a theory for everything. For all people and everything that happens. We have had Darwin and Einstein and Freud and people with literary theory and all the others. Frankly speaking, I believe that you are wrong. There is a theory of everything.

B. 'Theory of everything' is a facetious metaphor for a theory that combines all four known forces of nature, the electromagnetic one, the two subatomic forces called the strong and the weak force, and gravitation.

J. I can't help thinking that some people are like a force of nature.

B. That is outside our subject.

J. Sorry. But I must say that the names that you give to your forces are very bad to say the least. You have absolutely no imagination.

B. Names are inessential. The essential thing is that physicists know what they mean. Two of my forces could said to be nuclear after the nucleus. The weak and the strong nuclear force.

J. It is a little better but the public must have more than neutral names to attach their thoughts to.

B. One could say that the weak force keeps the nucleus together. The strong force protects the nucleus against strong radiation but not against very strong. Then the interior of the nucleus changes, the protons and neutrons flow together to a soup of quarks and gluons.

J. Excellent! Soup!

B. This means that very many quarks and gluons lie in disorder and tight together. As the molecules in water. We observe radiation from something that earlier was protons and now has changed to something else and must have a name. The word quark means a theoretical particle that can only be observed together with other quarks.

J. Fascinating. But can it be used for something?

B. No. We have to do with a state that can only last for a fraction of a second under the influence of extreme forces brought about by a collision.

J. So that were the two forces. And after that?

B. Electromagnetism and the nuclear forces are subject to a mathematical theory called the standard model.

J. Another neutral name saying nothing.

B. Once many physicists were responsible for the mathematical and physical parts of this model. So many that it was inconvenient to quote them all. Then the name became what it is.

J. I see. I feel uncomfortable that you mention the word mathematics. I was terrible in that subject at school.

B. It is not the first time that I hear this confession. With time one becomes insensitive to it. The task of mathematics is to give a strict frame that does not allow loose conjectures which destroy physics.

J. I am sorry about that. But what does your book say?

B. That if the standard model is extended to include also gravitation, only serious contradictions can result.

J. Why that?

B. It is explained in the book.

J. I can't take that as an answer. Say more.

B. I could say that the standard model cannot be combined with gravitation without exploding.

J. I hope it did not.

B. But it did. Under my eyes. But it was a logical explosion on paper and in my brain.

J. That cannot be understood.

B. Not verbally perhaps, but with a little imagination. It was only a personal experience.

J. And what are the consequences for the British people and for humanity?

B. None.

J. Do you think anyone would be interested?

B. No, the only thing of importance is the book where I have proved that the standard model and gravitation are incompatible.

J. Is anyone interested in that?

B. Everyone who tries to make a theory for everything.

J. You may be wrong.

B. This is an eventuality for every researcher.

J. But if what you did may be wrong, why should it be in the paper?

B. You came here. The editor who sent you tries to cover the frontier of research. Besides, if you do not write anything, nothing will appear in the paper.

J. Sorry, I take it back. I was stupid. But you must understand that you are not a very responsive person when it comes to interviews.

B. I am sorry. You could perhaps write about my hobby?

J. With pleasure. What is your hobby?

B. I share it with many. Bird-watching.

J. Yes, well I think we are ready now and I thank you very much.

The following account of this conversation appeared in the press the day after.

A discovery in physics

The walls of Professor Boriander's office are lined with books. His desk is clean except for a computer. The professor himself, in blue jeans and a green sweater, makes a youthful impression although retirement is approaching. We are going to talk about modern physics where Boriander recently made a breakthrough. He has proved that the much wanted theory of everything leads to contradictions. The professor himself, on the contrary, is not contradictory. His clear intellect illuminates our conversation when he gives me a lively description of the smaller parts of atoms, among others the enigmatic quarks, and explains that the name 'theory of everything' is a technical term which is used because so many were involved in the work that it was too much trouble to mention all of them. Therefore no one is mentioned. And it is perhaps best so now when the theory has been proved to be contradictory. Boriander describes his discovery as an explosion on paper and in the brain. But he is careful to point out that he, as all researchers, may be wrong. But we hope that time will prove him right.

J.

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COMMUNICATION III

12 Art and Science

Louise Larfeldt (L.), art professor and Patric Predient (P.), professor of chemistry, have both been engaged to appear in a popular radio program on Channel Four called Art and Science. Below they rehearse their future appearance.

L. I suggest that we start our rehearsal straight away. Call me Louise.

P. Thanks, I am simply Patric. Why did you accept to take part in the Art and Science series. It seems to me to be pure entertainment.

L. To me it is not only entertainment. Art and Science are indispensable to everybody. Without them we would not be human. Why did you accept?

P. By vanity. To be asked is a sign of appreciation which is difficult not to enjoy.

L. The same feeling bit me, too. Like you I'm only human. But in my work publicity does not hurt. When I think about our future performance I do not quite know how to start. Art and Science, painting for me and chemistry for you, seem to have nothing in common except the paint.

P. I am sure that we will have a moderator giving some kind of introduction where he says, roughly, that art and science are sisters in human culture. I have my own theory about that. I believe that the pair 'art and science' comes from the princely courts a long time ago. There art and science were both activities that were useful to the prince. Something like tokens of his princely might. For instance impressive works of art to show his good taste and science or something similar to show his spiritual powers. That is why art and science came together at a princely court. And now it is the state that adorns itself in the same way.

L. I do not believe you. Now that we live in a democracy, the prince is old hat.

P. If you excuse me, I want to insist. The state has taken over after the prince with about the same motives. The prestige that we, I mean art and science, once acquired as the finer parts of a princely culture still sticks to us. As just any chemist I would not have been invited to our program. But now I am a state official and a known scientist and also known to write in the press.

L. Your credentials are not too bad for what we are going to do.

P. Not bad at all. I admit that. They fit precisely.

L. But let us be a bit serious. In what way does the stuff we do have anything in common and in what way are we useful to each other?

P. We have not started yet. My speciality is nucleic acid. I am an organic chemist. This means that I have a vague connection with DNA, the new genetics, but only in a distant way. That is me.

L. And I am as established painter of the postmodern variety. To go with the times I began to do installations and succeeded well. Now, for a period, I am professor at distinguished art school. My students and I investigate reality and imagination in many seminar groups. My students also paint.

P. For the moment I agree with you that the paint is the only link between us. But this fact can only pass as a facetious remark in a conversation about art and science. We must in some way or other find a subject for discussion tying art and science together.

L. We could discuss conditions for research.

P. Not a stupid suggestion. Then we will be almost liberated from the attractions that made us eligible in the minds of those who run Art and Science. And we have to conceal our professional identities under a mask of experience and reason.

L. Please do not be so cynical. We do research all the time and gather a lot of experience.

P. Give me two examples.

L. We have seminars on subjects like this: 'When does a painting become a painting?' and 'When does reality ceases to be reality?'

P. But your questions do not have answers.

L. On the contrary. We ask them in connection with examples taken from our own experiences and our painting. You would be surprised to hear all the interesting arguments in such debates. Don't you have something similar?

P. No, I don't think so. Our problems are different. We must have large computer programs to master all the nucleic acids and their chemical compositions. It is for instance extremely difficult to get pure specimens. Our research deals partly with getting pure specimens, partly we worry about the interpretations of computer pictures. We do not worry about existence except for certain chemicals. I would be laughed down if I suggested a discussion with the theme *When does an experiment cease to be an experiment*?

L. But research is not only systematic work. It means more, for instance anxiety, thwarted hopes and sometimes success.

P. This is true, but where I am such things are kept strictly personal and have no chemical or human interest.

L. I think that you are wrong. Personal and individual reactions are extremely important in art. And why not in science? Personal experiences are all-important and even decisive for everybody.

P. If you do not mind I think that we have gotten nowhere with our comparisons. I mean that what we have to do during this session on Channel Four is to try to say something interesting. To make personal confessions about this and that is too common. It is better to say something about our subjects.

L. I tried but I did not hear much from you except protests.

P. Maybe, but I cannot go against the convictions that I got when working nucleic acids. But, I have an idea!

L. I can't wait.

P. We could try to discuss the part that our subjects play here in daily life in the beginning of the third millennium.

L. Agreed! I think that art is indispensable for modern man.

P. And I believe that the results of chemistry in the form of all new materials is equally indispensable. Our daily life is dominated by polymers.

L. What do you mean by that?

P. For a long time chemists have worked with long chains of molecules called polymers and this has given us plastic. The majority of things that we carry are made of plastic. Earlier the same things were made of burnt clay or iron. We live in the age of plastic. Five hundred years after us, archaeologists will baptize our time the older plastic age because pieces of plastic is all they find in their excavations. Organic material has disappeared and iron has turned to rust.

L. But plastic is neither science nor art.

P. It is not art and not science but plastic is a creation of science.

L. But I want that we shall talk about the spiritual and human side of science. And the social side, too.

P. I think that plastic has a lot to do with the social side. For instance in the third world where light plastic vessels have made life much brighter at the water wells. But I am afraid that the spiritual element that once was present in chemistry has disappeared. I mean when chemists thought about their subject in small laboratories or were happy at some discovery. All this has disappeared into the impenetrable prose cover of scientific journals.

L. That's a pity. We have tried to find something common to us both but we have not achieved much. We seem still to be where we were with the paint. Perhaps we shall need help.

P. Perhaps the moderator could do something. Let me imagine what he could say. So, when I speak now, I am the moderator and you have to answer and play your part.

L. That sounds good. Please start.

M. Tonight two distinguished scientists have agreed to come to talk about art and science, a subject of growing importance in our time where globalization and a dominating market threaten the soul of both art and science. My two guests are Louise Larfeldt, a famous painter and a professor at the Academy of the Free Arts, and Patric Predient, a world famous chemist and well known science popularizer. We welcome both of them. Perhaps I should start with *a question. How did you first get an idea of your future careers? Let me ask Louise first.*

L. Already as a young girl I felt an attraction to art and music and at first did not know what I should choose. My many visits to the great European museums finally led me to painting. This became for me the only way.

M. Thank you. And Patric, if I put the same question to you?

P. Curiously enough I also imagined a future as a musician, in my case the clarinet. But then I went to the university and chemistry took over.

M. Well, you are both musicians. Did you feel anything musical in the careers that you have chosen?

P. Chemistry reminds me in a way about the music of Bach. The two have something in common, namely a careful no-nonsense texture that is sometimes broken by strokes of genius.

M. And Louise, do you feel something like that?

L. For me a good painting is a piece of frozen music. I have felt that many times wen I have done something that I really liked.

M. Isn't it a wonderful thing that you both are musicians, heart and soul! How do combine this with your daily work?

L. Not difficult. Sometimes I play ABBA when my own inspiration fails.

P. And I use to hum Rule Britannia when my work seems to go astray. It cheers me up.

M. You are both scientists in your own way. How is it to do science these days. Does your research not suffer from the new restlessness and the globalization?

L. You are absolutely right that the aesthetical sciences are strongly dependent on research. Without it we would now paint like Delacroix. I can't say that the new restlessness has entered my creative work. I try by all means to keep it away.

P. I like to go to conferences and therefore I like the new restlessness. So far.

L. You were not so bad as a moderator. Let me also try.

P. OK.

S. You represent very different branches of science. Let me ask if you are aware of each other's work?

P. I do not know about painting in a precise way, but I have eyes to see and I am not insensible. The paintings of Velasquez in El Prado once made a very strong impression on me.

L. I also use my eyes. And when I see so many things in everyday life that are made of plastic, I think that the origin of all this is modern chemistry.

M. You really seem to know about each other. Let me ask whether your professions can give you fully emotional experiences?

P. In any case some kind of emotion. I am thinking of my feelings brought about by disappointment and success. They can sometimes fill my entire personality for days.

M. I did not mean that exactly. I meant feelings brought about by a sense of the unity of art and science in our culture.

L. It is precisely such feelings that overwhelm me almost every day. Art is an infinite source of elevated feelings. Not only the unity of thought and space. And the feeling of belonging to the universe.

P. You were not bad at all as moderator, Louise, although I think you were a bit too far out in the universe. Perhaps we could finish now. I thought that our problems were more or less solved by themselves now when have had a moderator and answered some questions. I am no longer nervous about our future performance.

L. Neither am I. But I do not think that we are done. Wasn't it so that we just unawares slipped into the question of how art and science hang together and how the two fertilize each other? We assumed that this was our subject. Without thinking as one does when writing a composition at school on a prescribed subject. The name of the our theme is Art and Science. Why not see it as Art *and* Science and make something out of the *and*.

P. I am thinking and I am ready to draw some conclusions that you may have already made. In order to appear, we do not have to construct connections between art and science except for the paint. We just talk about various things as they come along. And this is what we have done. We do not even need a moderator oozing kindness and good will. Each one speaks for himself. Simple comparisons appear by themselves in such conversations. And we understand each other without any forced comparisons. We have so much in common. Everything that made us to what we are. The same language, the same upbringing and the same country. We really understand each other.

L. You speak like a patriotic sociologist but I agree with what you say. If our conversation had come straight out live on the radio we may even had been a success. By the way, what did you think of me as a moderator?

P. I thought you were excellent.

L. And I that you were brilliant. Congratulations.

P. Thanks! See you later!

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