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Advances in Quantum Mechanics

Contemporary Trends and Open Problems

Springer

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Volume 18

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ISSN 2281-518X ISSN 2281-5198 (electronic)
Springer INdAM Series
ISBN 978-3-319-58903-9 ISBN 978-3-319-58904-6 (eBook)
DOI 10.1007/978-3-319-58904-6

Library of Congress Control Number: 2017942781

Printed on acid-free paper

This Springer imprint is published by Springer Nature
The registered company is Springer International Publishing AG
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

Preface

This volume is a collection of recent contributions and up-to-date surveys on many contemporary trends in the mathematics of quantum mechanics, and more generally on mathematical problems arising in quantum many-body dynamics, quantum graph theory, cold atoms and unitary gases. Special emphasis is devoted to development of the specific mathematical tools needed, including linear and non-linear Schrödinger equations, topological invariants, non-commutative geometry, resonances and operator extension theory.

Most of the contributors are leading international experts or recognised young researchers in mathematical physics, PDE theory and operator theory. The material that they present is the fruit of recent studies that have already become a reference in the community. The underlying motivation from condensed matter physics, solid state physics and ultra-cold atom physics, and the topicality of the research topics, give the volume a distinctive perspective at the edge of mathematics and physics.

A large part of the material was presented and discussed thoroughly on the occasion of the INdAM international meeting entitled "Contemporary Trends in the Mathematics of Quantum Mechanics", which took place in Rome from 4 to 8 July 2016 and which we had the honour of organising thanks to a very generous funding and most helpful logistic support from INdAM. The remainder of the material was produced as a follow-up to that meeting or as closely related work.

First and foremost, our thanks go to the scientific board of INdAM and the responsible administrative staff at the INdAM headquarters in Rome for providing such a stimulating atmosphere and all the necessary practical help. We would also like to warmly acknowledge all contributors and anonymous reviewers for their careful work and the quality of their reports. Finally, we extend our gratitude to the extremely supportive team of the INdAM Springer Series for their services throughout the editing and publishing process.

Trieste, Italy — Gianfausto Dell'Antonio
Trieste, Italy — Alessandro Michelangeli
April 2017

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About the Editors

Prof. Gianfausto Dell'Antonio's research focuses on axiomatic quantum field theory, local field theory, mathematics of quantum mechanics, critical point theory, stochastic processes, singular interactions,and many-body problems. He graduated in theoretical physics in Milan, was research associate in Copenhagen (Niels Bohr institute), Zurich (ETH), and Evanson (Northwestern), then professor of theoretical physics in Naples and professor of rational mechanics and mathematical physics at La Sapienza Rome. He held visiting professorships at the IHES Paris, Courant Institute NY, The University of Marseille Luminy, Bielefeld University (as a recipient of a von Humboldt prize), CERN, SISSA Trieste, and the Interdisciplinary Laboratory of the Accademia dei Lincei. He held also visiting positions at the IAS Princeton, Ecole Politechnique Paris, Paris Dauphine, Harvard University, and the Max Planck Institute inMunich.

Dr. Alessandro Michelangeli's research is in the field at the interface between mathematical physics, functional analysis and non-linear dispersive PDE, and operator theory, with a special focus on the mathematical methods for quantum mechanical and condensed matter systems. He graduated in theoretical physics in Pisa and in mathematical physics at SISSA Trieste, held faculty positions at the LMU Munich and SISSA Trieste, and visiting positions at the University of Cambridge, SISSA Trieste, and Bilkent.

Shell Interactions for Dirac Operators

Naiara Arrizabalaga

Abstract In this notes we gather the latest results on spectral theory for the coupling $H + V$, where $H = -i\alpha \cdot \nabla + m\beta$ is the free Dirac operator in $\mathbb{R}^3$, $m > 0$ and V is a measure-valued potential. The potentials under consideration are given in terms of surface measures on the boundary of bounded regular domains in $\mathbb{R}^3$. We give three main results. We study the self-adjointness. We give a criterion for the existence of point spectrum, with applications to electrostatic shell potentials, V_λ, which depend on a parameter $\lambda \in \mathbb{R}$. Finally, we prove an isoperimetric-type inequality for the admissible range of λ's for which the coupling $H + V_\lambda$ generates pure point spectrum in $(-m, m)$. The ball is the unique optimizer of this inequality.

Keywords Dirac operator • Self-adjoint extension • Shell interaction • Singular integral

1 Introduction and Main Results

The quantum mechanical model presented in these notes is a shell interaction for Dirac operators, which is nothing else than the free Dirac operator in $\mathbb{R}^3$ coupled with a measure-valued potential.

Given $m \geq 0$, the free Dirac operator in $\mathbb{R}^3$ is defined by $H = -i\alpha \cdot \nabla + m\beta$, where $\alpha = (\alpha_1, \alpha_2, \alpha_3)$,

$$\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} \quad \text{for } j = 1, 2, 3, \quad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \quad I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$
$$\text{and} \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1}$$

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A. Michelangeli, G. Dell'Antonio (eds.), *Advances in Quantum Mechanics*,
Springer INdAM Series 18, DOI 10.1007/978-3-319-58904-6_1

is the family of *Pauli matrices*. It is a first order symmetric differential operator that was introduced by Paul Dirac in 1929. The operator is a local version of $\sqrt{-\Delta + m^2}$ and satisfies

$$H^2 = (-\Delta + m^2)I_4, \tag{2}$$

which turns to be a very useful property. The equation associated to this operator describes a relativistic electron or positron which moves freely as there were no external forces nor other particles, and, has played a fundamental role in various areas of physics and mathematics.

In this work we show spectral properties of the coupling $H + V$ where V is a singular potential located at the boundary of a bounded regular domain. The first point is to construct a domain where these operators are self-adjoint. Secondly, we give a criterion for the existence of eigenvalues of $H + V$. This criterion is a kind of Birman-Schwinger principle adapted to our setting. We apply this criterion to electrostatic shell potentials, V_λ, where $\lambda \in \mathbb{R}$ is the coupling constant, for which we are able to prove more specific spectral properties. Finally, we study an isoperimetric-type inequality for the possible λ's for which the operator $H + V_\lambda$ have non trivial eigenvalues in $(-m, m)$. We also show that the ball is the unique optimizer of this inequality.

Note that one can take $m = 0$ in the definition of H, however, throughout these notes we assume $m > 0$ to allow the existence of a nontrivial pure point spectrum in the interval $(-m, m)$ for the corresponding couplings.

The results presented in these notes have been obtained in a joint work with Albert Mas and Luis Vega (see [1–3]).

1.1 Self-Adjointness for $H + V$

The problem of self-adjointness of Dirac operators has a long history starting in the early 1970s. In what respects to shell interactions, the case of the sphere was previously studied in [4] by J. Dittrich, P. Exner and P. Seba. Since the proofs for that case rely heavily on spherical symmetry and spherical harmonics, it is not possible to extend those arguments to a more general domains, as it is our case.

First, let us present our setting. The ambient Hilbert space is $L^2(\mathbb{R}^3, \mu)^4$ with respect to the Lebesgue measure μ. Given a bounded regular domain $\Omega \subset \mathbb{R}^3$ with boundary $\partial\Omega$ and surface measure σ, our aim is to find domains $D \subset L^2(\mathbb{R}^3, \mu)^4$ in which $H + V : D \to L^2(\mathbb{R}^3, \mu)^4$ is an unbounded self-adjoint operator, where H is defined in the sense of distributions and V is a suitable $L^2(\partial\Omega, \sigma)^4$-valued potential. To shorten notation we denote $L^2(\mathbb{R}^3, \mu)^4$ and $L^2(\partial\Omega, \sigma)^4$ by $L^2(\mathbb{R}^3)^4$ and $L^2(\sigma)^4$, respectively. We construct the domain D as follows: by assumption, V is $L^2(\sigma)^4$-valued. Thus, given $\varphi \in D$, we can write $V(\varphi) = -g$ in the sense of distributions for some $g \in L^2(\sigma)^4$. Moreover, since $(H + V)(\varphi) \in L^2(\mathbb{R}^3)^4$, we can also write $(H + V)(\varphi) = G$ for some $G \in L^2(\mathbb{R}^3)^4$. Therefore, $H(\varphi) = G + g$ in the sense of distributions, and therefore, φ should be the convolution $\phi * (G + g)$, where

$$\phi(x) = \frac{e^{-m|x|}}{4\pi|x|}\left(m\beta + (1 + m|x|)\ i\alpha \cdot \frac{x}{|x|^2}\right)$$

is a fundamental solution of H. This fundamental solution can be easily computed by using (2). In particular,

$$D \subset \{\varphi = \phi * (G + g) : G \in L^2(\mathbb{R}^3)^4,\ g \in L^2(\sigma)^4\} \quad \text{and} \\ V(\varphi) = -g \quad \text{for all } \varphi = \phi * (G + g) \in D. \tag{3}$$

To ensure that $H+V$ is self-adjoint on D, we need to impose some relations between G and g with the aid of bounded self-adjoint operators $\Lambda : L^2(\sigma)^4 \to L^2(\sigma)^4$. In other words, given suitable Λ's, following (3) we find domains D_Λ (which depend on Λ) where $H + V$ is self-adjoint.

We consider the potential V given by (3) as a generic potential since it seems to be prescribed from the beginning as $V(\varphi) = -g$ for all $\varphi = \phi * (G + g) \in D_\Lambda$, so V is independent of Λ. Hence, if we want to work with a given boundary potential, that we will denote by V_σ, the key idea to construct a domain where $H + V_\sigma$ is self-adjoint is to find a particular bounded self-adjoint operator Λ so that $V_\sigma(\varphi) = -g$ for all $\varphi \in D_\Lambda$.

Let us roughly mention the idea behind the generic potential V given by (3). If we know that the gradient of a function φ has an absolutely continuous part G and a singular part g supported on $\partial\Omega$ (in our setting, $V(\varphi) \in L^2(\sigma)^4$ and $(H + V)(\varphi) \in L^2(\mathbb{R}^3)^4$), then φ must have a jump across $\partial\Omega$, and this jump completely determines the singular part of the gradient (that is, the jump determines the value $V(\varphi)$). For a given potential V_σ, one manages to define a suitable domain D such that, for any $\varphi \in D$, the singular part which comes from the gradient on the jump of φ across $\partial\Omega$ agrees with $-V_\sigma(\varphi)$. From now on we will simply denote by V the given boundary potential under study.

Observe that H, which is symmetric and initially defined in $\mathscr{C}_c^\infty(\mathbb{R}^3)^4$ ($\mathbb{C}^4$-valued functions in $\mathbb{R}^3$ which are $\mathscr{C}^\infty$ and with compact support), can be extended by duality to the space of distributions with respect to the test space $\mathscr{C}_c^\infty(\mathbb{R}^3)^4$ and, in particular, it can be defined on $\mathscr{X} = \left\{G\mu + g\sigma :\ G \in L^2(\mathbb{R}^3)^4,\ g \in L^2(\sigma)^4\right\}$.

In order to construct a domain of definition where $H + V$ is self-adjoint, we have to consider the trace operator on $\partial\Omega$. So, to ensure that the trace operator is well defined, we need to use the following lemma: if $G \in L^2(\mathbb{R}^3)^4$, then $\phi * G \in W^{1,2}(\mathbb{R}^3)^4$ and $(\phi * G)_{|\partial\Omega} \in L^2(\sigma)^4$ (see [1]).

Given an operator between vector spaces $S : X \to Y$, denote $\mathrm{kr}(S) = \{x \in X : S(x) = 0\}$ and $\mathrm{rn}(S) = \{S(x) \in Y :\ x \in X\}$.

Theorem 1.1 *Let $\Lambda : L^2(\sigma)^4 \to L^2(\sigma)^4$ be a bounded operator. Set*

$$D = \{\phi * (G + g) : G\mu + g\sigma \in \mathscr{X},\ (\phi * G)_{|\partial\Omega} = \Lambda(g)\} \subset L^2(\mathbb{R}^3)^4$$

and $H+V$ *on* D*, where* $V(\varphi) = -g\sigma$ *and* $(H+V)(\varphi) = G$ *for all* $\varphi = \phi*(G+g) \in D$*. If* Λ *is self-adjoint and* $\mathrm{rn}(\Lambda)$ *is closed, then* $H + V : D \to L^2(\mathbb{R}^3)^4$ *is an essentially self-adjoint operator. Moreover, if* $\{\phi * h : h \in \mathrm{kr}(\Lambda)\}$ *is closed in* $L^2(\mathbb{R}^3)^4$*, then* $H + V$ *is self-adjoint.*

Furthermore, if Λ is self-adjoint and semi-Fredholm, then $H + V$ is self-adjoint. We study other differential operators and measures and other relations between $(\phi * G)_{|\partial\Omega}$ and g, but we consider that they are not relevant for the purpose of these notes. In [7] (see also [8, Sect. 2]), A. Posilicano gives a more general result. There the author provides, in a very general framework, all self-adjoint extensions of symmetric operators obtained by restricting a self-adjoint operator to a dense subspace of the domain. See [1] for the complete details.

1.2 Point Spectrum for $H + V$

The natural question that comes to our mind after studying the self-adjointness of shell interactions for Dirac operators is: what can we say about their point spectrum? In this section, we show a criterion for the existence of eigenvalues in $(-m, m)$ for $H + V$. This criterion is a kind of Birman-Schwinger principle adapted to our setting. Afterwards, we show some applications to the case of electrostatic shell potentials.

For convenience, set $\Omega = \Omega_+$. Let $\partial\Omega$ be the boundary of a bounded Lipschitz domain $\Omega_+ \subset \mathbb{R}^3$, let σ and N be the surface measure and outward unit normal vector field on $\partial\Omega$, respectively, and set $\Omega_- = \mathbb{R}^3 \setminus \overline{\Omega_+}$, so $\partial\Omega = \partial\Omega_\pm$. Note that σ is 2-dimensional. Since we are not interested in optimal regularity assumptions, for the sequel we assume that $\partial\Omega$ is of class $\mathscr{C}^2$.

Before stating the main result of this subsection, we need to consider some properties of operators defined only at the boundary of the domain. Let $a \in (-m, m)$, a fundamental solution of $H - a$ for $x \in \mathbb{R}^3 \setminus \{0\}$ is given by

$$\phi^a(x) = \frac{e^{-\sqrt{m^2-a^2}|x|}}{4\pi|x|}\left(a + m\beta + \left(1 + \sqrt{m^2 - a^2}|x|\right) i\alpha \cdot \frac{x}{|x|^2}\right).$$

Lemma 1.2 *Given* $g \in L^2(\sigma)^4$ *and* $x \in \partial\Omega$*, set*

$$C^a_\sigma(g)(x) = \lim_{\epsilon \searrow 0} \int_{|x-z|>\epsilon} \phi^a(x - z)g(z)\, d\sigma(z)$$

and

$$C^a_\pm(g)(x) = \lim_{\Omega_\pm \ni y \xrightarrow{nt} x} (\phi^a * g\sigma)(y),$$

where $\Omega_\pm \ni y \xrightarrow{nt} x$ *means that* $y \in \Omega_\pm$ *tends to* $x \in \partial\Omega$ *non-tangentially. Then, the Cauchy type singular operator* C^a_σ *and the operators* $C^a_\pm$ *are bounded and linear* *in $L^2(\sigma)^4$. Moreover, the following holds:*

(i) $C^a_\pm = \mp\frac{i}{2}(\alpha\cdot N) + C^a_\sigma$ *(Plemelj–Sokhotski jump formulae),*
(ii) *for any* $a \in [-m, m]$, C^a_σ *is self-adjoint and* $-4(C^a_\sigma(\alpha\cdot N))^2 = I_4$.

The following criterion relates the eigenvalues of $H + V$ with a spectral property of bounded operators in $L^2(\sigma)^4$ mentioned in Lemma 1.2, that is, it relates a problem in $\mathbb{R}^3$ with a problem settled exclusively on $\partial\Omega$.

Proposition 1.3 *Let* $H + V$ *be as in* Theorem 1.1. *Given* $a \in (-m, m)$, *there exists* $\varphi = \phi * (G+g) \in D$ *such that* $(H+V)(\varphi) = a\varphi$ *if and only if* $\Lambda(g) = (C^a_\sigma - C_\sigma)(g)$ *and* $G = a\phi^a * g$. *Therefore,* $\mathrm{kr}(H+V-a) \neq 0$ *if and only if* $\mathrm{kr}(\Lambda + C_\sigma - C^a_\sigma) \neq 0$.

1.2.1 Applications to Electrostatic Shell Potentials

In this summary we are particularly interested in the case of electrostatic shell potentials as the ones defined in the theorem below, V_λ. These potentials are also known as δ-shell potentials. It is for these potentials for which we give the isoperimetric-type inequality detailed in the next subsection.

Theorem 1.4 *Let* $\lambda \in \mathbb{R}\setminus\{0\}$ *and* $a \in (-m, m)$. $D = \{\varphi = \phi * (G + g) : (\phi * G)|_{\partial\Omega} = -(1/\lambda + C_\sigma)g\}$, *and* $V_\lambda(\varphi) = \frac{\lambda}{2}(\varphi_+ + \varphi_-)$, *where* $\varphi_\pm$ *are the boundary values of* φ *when approaching* $\partial\Omega$ *from* Ω_+ *or* Ω_-.

(i) $H + V_\lambda$ *defined on* D *is self-adjoint for all* $\lambda \neq \pm 2$.
(ii) $Ker(H + V_\lambda - a) \neq 0$ *iff* $Ker(1/\lambda + C^a_\sigma) \neq 0$.
(iii) $H + V_\lambda$ *and* $H + V_{-4/\lambda}$ *have the same eigenvalues in* $[-m, m]$.
(iv) *If* $|\lambda| \notin [1/\|C^a_\sigma\|, 4\|C^a_\sigma\|]$, *then* $Ker(H + V_\lambda - a) = 0$.
(v) *If* $|\lambda| \notin [1/C, 4C]$, *where* $C = \sup_{a\in(-m,m)} \|C^a_\sigma\| < \infty$, *then* $H + V_\lambda$ *has no eigenvalues in* $(-m, m)$.
(vi) *If* Ω_- *is connected, then* $H + V_\lambda$ *has no eigenvalues in* $\mathbb{R}\setminus[-m, m]$.

The last theorem shows that there are a lower and upper thresholds on the possible values of λ in order to have non trivial eigenvalues in $(-m, m)$. This is different from what happens with other similar potentials, such as the Coulomb potential or the characteristic function of a ball. The Coulomb potential, for example, generates eigenvalues for any small λ. The self-adjointness for the cases $\lambda = \pm 2$ is currently under study.

1.3 Isoperimetric-Type Inequality

Previously, we found that for the case of electrostatic shell potentials there is no possible φ verifying

$$(H + V_\lambda)(\varphi) = a\varphi \tag{4}$$

for any $a \in (-m, m)$ if $|\lambda|$ is either too big or too small. More precisely, we showed that there exist upper and lower thresholds $\lambda_u(\partial\Omega)$ and $\lambda_l(\partial\Omega)$, respectively, with $0 < \lambda_l(\partial\Omega) \leq 2 \leq \lambda_u(\partial\Omega)$ and such that if $|\lambda| \notin [\lambda_l(\partial\Omega), \lambda_u(\partial\Omega)]$ then there exists no nontrivial φ verifying (4) for some $a \in (-m, m)$.

The main purpose of this section is to determine how small can $[\lambda_l(\partial\Omega), \lambda_u(\partial\Omega)]$ be under some constraint on the size of $\partial\Omega$ and/or Ω.

Given a compact set $E \subset \mathbb{R}^3$, the *Newtonian capacity* of E (sometimes referred in the literature as *electrostatic* or *harmonic capacity*) is defined by

$$\mathrm{Cap}(E) = \left(\inf_{\nu} \iint \frac{d\nu(x)\, d\nu(y)}{4\pi|x-y|}\right)^{-1},$$

where the infimum is taken over all probability Borel measures ν supported in E. Sometimes in the literature, the 4π appearing in the definition of $\mathrm{Cap}(E)$ is changed by another precise constant. For the case of open sets $U \subset \mathbb{R}^3$, one defines

$$\mathrm{Cap}(U) = \sup\{\mathrm{Cap}(E) :\, E \subset U,\, E \text{ compact}\}.$$

Let us mention some examples of constraints where the Newtonian capacity appears. Let $\Omega \subset \mathbb{R}^3$ be a bounded smooth domain. On the one hand, we have the following isoperimetric inequality

$$36\pi\,\mathrm{Vol}(\Omega)^2 \leq \mathrm{Area}(\partial\Omega)^3.$$

On the other hand, the Pólya-Szegö inequality, [6], asserts that

$$\mathrm{Cap}(\overline{\Omega}) \geq 2(6\pi^2\mathrm{Vol}(\Omega))^{1/3},$$

where ν is the probability measure and $\mathrm{supp}(\nu) \subset \overline{\Omega}$. In both cases, equality holds if and only if Ω is a ball. Our main result in this sense is the following one.

Theorem 1.5 *Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with smooth boundary and assume that*

$$m\,\frac{\mathrm{Area}(\partial\Omega)}{\mathrm{Cap}(\Omega)} > \frac{1}{4\sqrt{2}}. \tag{5}$$

Then

$$\sup\{|\lambda| :\, \mathrm{kr}(H + V_\lambda - a) \neq 0 \text{ for some } a \in (-m, m)\}$$
$$\geq 4\left(m\,\frac{\mathrm{Area}(\partial\Omega)}{\mathrm{Cap}(\Omega)} + \sqrt{m^2\left(\frac{\mathrm{Area}(\partial\Omega)}{\mathrm{Cap}(\Omega)}\right)^2 + \frac{1}{4}}\right),$$

$$\inf\{|\lambda| : \operatorname{kr}(H + V_\lambda - a) \neq 0 \textit{ for some } a \in (-m, m)\}$$
$$\leq 4\left(-m\,\frac{\text{Area}(\partial\Omega)}{\text{Cap}(\Omega)} + \sqrt{m^2\left(\frac{\text{Area}(\partial\Omega)}{\text{Cap}(\Omega)}\right)^2 + \frac{1}{4}}\right).$$

In both cases, the equality holds if and only if Ω is a ball.

2 On the Proof of the Main Results

For the sake of shortness we focus our attention on the proof of the newest result, Theorem 1.5. See [1] for the details on the proof of Theorem 1.1 and [2] for Proposition 1.3 and Theorem 1.4.

There are three key steps on the proof of Theorem 1.5. First, recall that this result is for electrostatics shell potentials. Thus, the starting point is Theorem1.4 (ii), where we relate (4) with the existence of a nontrivial eigenvalue $c(a)$ of C^a_σ. Once we have this relation, we show that $c(a)$ is a monotone function of $a \in (-m, m)$. This has important consequences because it reduces the problem to the study of the limiting cases $a = \pm m$. Thanks to the well-known properties of the Cauchy operator stated in Lemma 1.2, it is sufficient to consider just the case $a = m$. Hence, it is enough to study $Ker(1/\lambda + C^m_\sigma)$. The next step is to prove that solving our optimization problem (to find the optimal λ for which $Ker(1/\lambda + C^m_\sigma) \neq 0$) is equivalent to minimizing, in terms of Ω, the infimum over all $\lambda > 0$ such that

$$\left(\frac{4}{\lambda}\right)^2 \int_{\partial\Omega} |W(f)|^2\, d\sigma + \frac{8m}{\lambda} \int_{\partial\Omega} K(f)\cdot \overline{f}\, d\sigma \leq \int_{\partial\Omega} |f|^2\, d\sigma, \tag{6}$$

for all $f \in L^2(\sigma)^2$. It is to this infimum λ to which we prove the isoperimetric-type inequality in Theorem 1.5. Finally, we write the isoperimetric-type inequality in terms of area and capacity.

2.1 Monotonicity

The following lemma contains the monotonicity property mentioned above.

Lemma 2.1 *Given $a \in [-m, m]$, the eigenvalues of C^a_σ form a finite or countable sequence $\emptyset \neq \{c_j(a)\}_j \subset \mathbb{R}$, with $1/4$ being the only possible accumulation point of $\{c_j(a)^2\}_j$. Moreover, $\frac{d}{da}\, c_j(a) > 0$ for all $a \in (-m, m)$ and all j.*

As a consequence, given $a \in (-m, m)$, the set of real λ's such that $\operatorname{kr}(H + V_\lambda - a) \neq 0$ form a finite or countable sequence $\emptyset \neq \{\lambda_j(a)\}_j \subset \mathbb{R}$, with 4 being the only possible accumulation point of $\{\lambda_j(a)^2\}_j$. Furthermore, $\lambda_j(a)$ is a strictly monotonous increasing function of $a \in (-m, m)$ for all j.

For any $a \in [-m, m]$, the existence of the sequence $\emptyset \neq \{c_j(a)\}_j \subset \mathbb{R}$ stated in the lemma and its possible accumulation point are guaranteed by the self-adjointness of C_σ^a and the fact that if we define $\Lambda_\pm^a = 1/\lambda \pm C_\sigma^a$, then

$$\Lambda_+^a \Lambda_-^a = \frac{1}{\lambda^2} - (C_\sigma^a)^2 = \frac{1}{\lambda^2} - \frac{1}{4} - C_\sigma^a(\alpha \cdot N)\{\alpha \cdot N, C_\sigma^a\},$$

where $C_\sigma^a(\alpha \cdot N)\{\alpha \cdot N, C_\sigma^a\}$ is a compact operator and self-adjoint. We want to study $\partial_a c_j(a)$. We denote $\partial_a \equiv \frac{d}{da}$ to shorten. Let $g_j(a) \in L^2(\sigma)^4$ be such that $\|g_j(a)\|_\sigma = 1$ and

$$C_\sigma^a(g_j(a)) = c_j(a) g_j(a). \tag{7}$$

To differentiate $c_j(a)$ with respect to a, we take the scalar product of (7) with $g_j(a)$, so

$$c_j(a) = \langle c_j(a) g_j(a), g_j(a)\rangle_\sigma = \langle C_\sigma^a(g_j(a)), g_j(a)\rangle_\sigma.$$

Thus, at a formal level and by using that C_σ^a is self-adjoint,

$$\partial_a c_j(a) = \langle (\partial_a C_\sigma^a)(g_j(a)), g_j(a)\rangle_\sigma + 2\mathrm{Re}\langle \partial_a g_j(a), C_\sigma^a(g_j(a))\rangle_\sigma. \tag{8}$$

Since $\|g_j(a)\|_\sigma = 1$ for all $a \in (-m, m)$, then (7) gives

$$0 = c_j(a)\partial_a \langle g_j(a), g_j(a)\rangle_\sigma = 2\mathrm{Re}\langle \partial_a g_j(a), C_\sigma^a(g_j(a))\rangle_\sigma.$$

Hence, we obtain $\partial_a c_j(a) = \langle (\partial_a C_\sigma^a)(g_j(a)), g_j(a)\rangle_\sigma$.

To justify the above computations, in particular in what respects to the issue of the principal value in the definition of C_σ^a, one can decompose the kernel

$$\phi^a(x) = \frac{e^{-\sqrt{m^2-a^2}|x|}}{4\pi|x|}\left(a + m\beta + i\sqrt{m^2-a^2}\,\alpha \cdot \frac{x}{|x|}\right) + \frac{e^{-\sqrt{m^2-a^2}|x|} - 1}{4\pi} i\left(\alpha \cdot \frac{x}{|x|^3}\right) + \frac{i}{4\pi}\left(\alpha \cdot \frac{x}{|x|^3}\right).$$

Note that the principal value only concerns to the last term, since the other two are absolutely integrable on $\partial\Omega$ and actually define compact operators, but the last one does not depend on a. At this point, standard arguments in perturbation theory allow us to justify the formal computations carried out above concerning ∂_a.

The next step is to understand the operator $\partial_a C_\sigma^a$. Since C_σ^a is defined as the convolution operator on $\partial\Omega$ with the fundamental solution of $H - a$, and formally $\partial_a((H-a)^{-1}) = (H-a)^{-2}$, then, as we may guess, $\partial_a C_\sigma^a$ is defined as the convolution operator on $\partial\Omega$ with the fundamental solution of $(H-a)^2$. In the following lines, we are going to prove the details of this argument. We can easily compute

$$\partial_a(\phi^a(x)) = \frac{ae^{-\sqrt{m^2-a^2}|x|}}{4\pi\sqrt{m^2-a^2}}\left(a + m\beta + i\sqrt{m^2-a^2}\,\alpha\cdot\frac{x}{|x|}\right) + \frac{e^{-\sqrt{m^2-a^2}|x|}}{4\pi|x|}. \tag{9}$$

Since $-i\alpha\cdot\nabla(e^{-\sqrt{m^2-a^2}|x|}) = i\sqrt{m^2-a^2}e^{-\sqrt{m^2-a^2}|x|}\,\alpha\cdot\frac{x}{|x|}$, then,

$$\partial_a(\phi^a(x)) = a\,(H+a)\,\frac{e^{-\sqrt{m^2-a^2}|x|}}{4\pi\sqrt{m^2-a^2}} + \frac{e^{-\sqrt{m^2-a^2}|x|}}{4\pi|x|}. \tag{10}$$

A simple calculation shows that

$$(-\Delta + m^2 - a^2)\frac{e^{-\sqrt{m^2-a^2}|x|}}{8\pi\sqrt{m^2-a^2}} = \frac{e^{-\sqrt{m^2-a^2}|x|}}{4\pi|x|}, \tag{11}$$

which combined with (10) and using that $-\Delta + m^2 - a^2 = (H-a)(H+a)$, yields

$$\partial_a(\phi^a(x)) = (H+a)^2\,\frac{e^{-\sqrt{m^2-a^2}|x|}}{8\pi\sqrt{m^2-a^2}}. \tag{12}$$

By using that $(4\pi|x|)^{-1}e^{-\sqrt{m^2-a^2}|x|}$ is a fundamental solution of $-\Delta + m^2 - a^2$ and that $(H-a)^2(H+a)^2 = (-\Delta + m^2 - a^2)^2$, because $-\Delta + m^2 - a^2$ commutes with $H+a$, then, we finally deduce that $(H-a)^2\,\partial_a(\phi^a(x)) = \delta_0$, which means that $\partial_a(\phi^a(x))$ is a fundamental solution of $(H-a)^2$, and $\partial_a C_\sigma^a$ corresponds to the operator of convolution on $\partial\Omega$ with this kernel. Note that $\partial_a(\phi^a(x)) = O(1/|x|)$ for $|x|\to 0$, so in particular $\partial_a C_\sigma^a$ is compact in $L^2(\sigma)^4$.

Given $g \in L^2(\sigma)^4$, set

$$u(x) = \int \partial_a(\phi^a(x-y))g(y)\,d\sigma(y) \qquad \text{for } x \in \mathbb{R}^3,$$

so $u = (\partial_a C_\sigma^a)(g)$ on $\partial\Omega$. Using (12), that $-\Delta + m^2 - a^2$ and $H+a$ commute and (11), we see that for any $x \in \mathbb{R}^3 \setminus \partial\Omega$,

$$(H-a)u(x) = \int (H_x - a)\partial_a(\phi^a(x-y))g(y)\,d\sigma(y) = \phi^a * (g)(x). \tag{13}$$

H_x denote the Dirac operator acting as a derivative on the x variable. Since ϕ^a is a fundamental solution of $H-a$, we see from (13) that $(H-a)^2u = 0$ outside $\partial\Omega$.

From Lemma 1.2(i), we have $g = i(\alpha\cdot N)(C_+^a(g) - C_-^a(g))$. Therefore, using the divergence theorem for $H-a$, that $(H-a)\phi^a * (g) = 0$ outside $\partial\Omega$ and (13), we finally get

$$\langle(\partial_a C_\sigma^a)(g), g\rangle_\sigma = \int_{\mathbb{R}^3\setminus\partial\Omega} |\phi^a * (g)|^2\, d\mu. \tag{14}$$

Thanks to the Plemelj–Sokhotski jump formulae from Lemma 1.2(i), we see that if $g \in L^2(\sigma)^4$ is such that $\phi^a * (g) = 0$ in $\mathbb{R}^3 \setminus \partial\Omega$ then $C_\pm^a(g) = 0$, and thus $g = 0$. Therefore, applying (14) to $g_j(a)$ and plugging it into

$$\partial_a c_j(a) = \langle(\partial_a C_\sigma^a)(g_j(a)), g_j(a)\rangle_\sigma$$

yields

$$\partial_a c_j(a) = \langle(\partial_a C_\sigma^a)(g_j(a)), g_j(a)\rangle_\sigma = \int_{\mathbb{R}^3\setminus\partial\Omega} |\phi^a * (g_j(a))|^2\, d\mu > 0.$$

Finally, by setting $c_j(a) = -1/\lambda_j(a)$ we see that $\lambda_j(a)$ is a strictly monotonous increasing function of $a \in (-m, m)$ for all j. This finishes the proof of the lemma.

From Theorem1.4 (ii) we know that the study of the eigenvalues of $H + V_\lambda$ is equivalent to the study of eigenvalues of C_σ^a, and from the previous result the eigenvalues of C_σ^a are a monotonous increasing function of a. Therefore, this reduces the problem to the study of $a = \pm m$. Moreover, by using the properties on Lemma 1.2, it is sufficient to consider just the case $a = m$. Therefore, the problem has been reduced to the study of $\mathrm{kr}(1/\lambda + C_\sigma^m) \neq 0$.

2.2 *Quadratic Forms*

Let us introduce some bounded operators defined exclusively on the boundary of the domain. For $a \in \mathbb{R}$ and $\sigma = (\sigma_1, \sigma_2, \sigma_3)$, where the σ_j's compose the family of Pauli matrices introduced in (1), define the kernels

$$k^a(x) = \frac{e^{-\sqrt{m^2-a^2}|x|}}{4\pi|x|} I_2 \quad \text{and} \quad w^a(x) = \frac{e^{-\sqrt{m^2-a^2}|x|}}{4\pi|x|^3}\left(1 + \sqrt{m^2-a^2}|x|\right) i\sigma\cdot x$$

for $x \in \mathbb{R}^3 \setminus \{0\}$. Given $f \in L^2(\sigma)^2$ and $x \in \partial\Omega$, set

$$K^a(f)(x) = \int k^a(x-z) f(z)\, d\sigma(z) \text{ and } W^a(f)(x) = \lim_{\epsilon\searrow 0} \int_{|x-z|>\epsilon} w^a(x-z) f(z)\, d\sigma(z).$$

That K^a and W^a are bounded operators in $L^2(\sigma)^2$ can be verified similarly to the case of C^a_σ in $L^2(\sigma)^4$, we omit the details. Moreover, note that

$$C^a_\sigma = \begin{pmatrix} (a+m)K^a & W^a \\ W^a & (a-m)K^a \end{pmatrix}. \tag{15}$$

For any $a \in [-m, m]$, K^a is positive and both K^a and the singular integral operator W^a are self-adjoint. For simplicity of notation, we write k, w, K and W instead of k^m, w^m, K^m and W^m, respectively. Thus, the study of $Ker(1/\lambda + C^m_\sigma) \neq 0$ is equivalent to find $\lambda \in \mathbb{R}$ and $u, h \in L^2(\sigma)^2$ such that

$$\begin{cases} 2mK(u) + W(h) = -u/\lambda, \\ \qquad\qquad\;\; W(u) = -h/\lambda. \end{cases}$$

Now by using the properties

$$\{(\sigma \cdot N)K, (\sigma \cdot N)W\} = 0 \quad \text{and} \quad [(\sigma \cdot N)W]^2 = -1/4, \tag{16}$$

we get $u = (4/\lambda)(\sigma \cdot N)W(\sigma \cdot N)(h)$. Plugging u into the first equation we obtain that there exists $f \in L^2(\sigma)^2, f \neq 0$ such that

$$\left(-\frac{8m}{\lambda}K + 1 - \frac{16}{\lambda^2}W^2\right) f = 0.$$

Multiply by $\overline{f}$, integrate with respect to σ and we get

$$\left(\frac{4}{\lambda}\right)^2 \int |W(f)|^2 \, d\sigma + \frac{8m}{\lambda} \int K(f) \cdot \overline{f} \, d\sigma = \int |f|^2 \, d\sigma,$$

where the second term on the left hand side is positive. Thus, the quadratic form is decreasing for $\lambda > 0$. As a consequence we have

$$\lambda_\Omega = \inf \left\{ \lambda > 0 : \left(\frac{4}{\lambda}\right)^2 \int |W(f)|^2 \, d\sigma + \frac{8m}{\lambda} \int K(f) \cdot \overline{f} \, d\sigma \leq \int |f|^2 \, d\sigma, \right\}$$

for all $f \in L^2(\sigma)^2$.

These arguments lead us to the next theorem, that is a key ingredient to derive the isoperimetric-type inequalities contained in Theorem 1.5. It gives the connection between the admissible λ's that generate eigenvalues of $C^{\pm m}_\sigma$ with the optimal constant of the inequality (17).

Theorem 2.2 *Let λ_Ω be the infimum over all $\lambda > 0$ such that*

$$\left(\frac{4}{\lambda}\right)^2 \int |W(f)|^2\, d\sigma + \frac{8m}{\lambda} \int K(f) \cdot \overline{f}\, d\sigma \le \int |f|^2\, d\sigma \tag{17}$$

for all $f \in L^2(\sigma)^2$. Then,

(i) $4\left(m\|K\|_\sigma + \sqrt{m^2\|K\|_\sigma^2 + 1/4}\right) \le \lambda_\Omega \le 4\left(m\|K\|_\sigma + \sqrt{m^2\|K\|_\sigma^2 + \|W\|_\sigma^2}\right)$,
(ii) *If $\lambda > 0$ is such that $\mathrm{kr}(1/\lambda + C_\sigma^m) \neq 0$ then $\lambda \le \lambda_\Omega$,*
(iii) *If $\lambda = \lambda_\Omega > 2\sqrt{2}$ then the equality holds, and the minimizers of (17) give rise to functions in $\mathrm{kr}(1/\lambda_\Omega + C_\sigma^m)$ and vice versa.*

For the first part of the theorem, we denote by $A(\lambda, f)$ the left hand side of (17) for a given $\lambda > 0$ and $f \in L^2(\sigma)^2$. Note that

$$A(\lambda, f) \le \left(\left(\frac{4\|W\|_\sigma}{\lambda}\right)^2 + \frac{8m\|K\|_\sigma}{\lambda}\right)\|f\|_\sigma^2. \tag{18}$$

Hence, if $\lambda \ge 4\left(m\|K\|_\sigma + \sqrt{m^2\|K\|_\sigma^2 + \|W\|_\sigma^2}\right)$ then (18) yields $A(\lambda, f) \le \|f\|_\sigma^2$ for all $f \in L^2(\sigma)^2$, which in turn implies that $\lambda_\Omega \le 4\left(m\|K\|_\sigma + \sqrt{m^2\|K\|_\sigma^2 + \|W\|_\sigma^2}\right)$.

The inequality from below is a bit more involved. Let $\lambda > 0$ be such that

$$A(\lambda, f) \le \|f\|_\sigma^2 \qquad \text{for all } f \in L^2(\sigma)^2. \tag{19}$$

If we set $h = \frac{4}{\lambda}(\sigma\cdot N)W(f) \in L^2(\sigma)^2$, then $f = -\lambda(\sigma\cdot N)W(h)$ by (16). Furthermore,

$$\int |W(f)|^2\, d\sigma = \left(\frac{\lambda}{4}\right)^2 \int |h|^2\, d\sigma \quad \text{and} \quad \int |f|^2\, d\sigma = \lambda^2 \int |W(h)|^2\, d\sigma. \tag{20}$$

Moreover, using (16) again,

$$\int K(f) \cdot \overline{f}\, d\sigma = \lambda^2 \int K(\sigma \cdot N)W(h) \cdot \overline{(\sigma \cdot N)W(h)}\, d\sigma = \frac{\lambda^2}{4} \int K(h) \cdot \overline{h}\, d\sigma. \tag{21}$$

Gathering (19) with (20) and (21) yields

$$\int |h|^2\, d\sigma + 2m\lambda \int K(h) \cdot \overline{h}\, d\sigma \le \lambda^2 \int |W(h)|^2\, d\sigma \tag{22}$$

for all $h \in L^2(\sigma)^2$. If we multiply (22) by $16/\lambda^4$ we get

$$\frac{16}{\lambda^4} \int |f|^2\, d\sigma + \frac{32m}{\lambda^3} \int K(f) \cdot \overline{f}\, d\sigma \le \frac{16}{\lambda^2} \int |W(f)|^2\, d\sigma$$

for all $f \in L^2(\sigma)^2$, which added to (19) gives

$$2m \int K(f) \cdot \overline{f}\, d\sigma \leq \left(\frac{\lambda}{4} - \frac{1}{\lambda}\right) \int |f|^2\, d\sigma \qquad \text{for all } f \in L^2(\sigma)^2.$$

Since K is bounded, positive and self-adjoint, we see from the above inequality that

$$2m\|K\|_\sigma = 2m \sup_{\|f\|_\sigma = 1} \int K(f) \cdot \overline{f}\, d\sigma \leq \frac{\lambda}{4} - \frac{1}{\lambda},$$

which in turn is equivalent to $\lambda^2 - 8m\|K\|_\sigma \lambda - 4 \geq 0$, since $\lambda > 0$ by assumption. Therefore, we must have $\lambda \geq 4\big(m\|K\|_\sigma + \sqrt{m^2\|K\|_\sigma^2 + 1/4}\big)$ for all $\lambda > 0$ satisfying (19). This gives the desired inequality from below for λ_Ω, and finishes the proof of (*i*). Observe that this lower bound for λ_Ω is strictly greater than 2 because $\|K\|_\sigma > 0$. The proof of (ii) comes from the arguments presented before the theorem. And, for the last part, since K is positive, $A(\lambda, f)$ is a non-increasing function of $\lambda > 0$ for all $f \in L^2(\sigma)^2$. By the definition of λ_Ω, this monotony implies that (17) holds for all $\lambda \geq \lambda_\Omega$ and it is sharp for $\lambda = \lambda_\Omega$. It remains to be shown that if $\lambda_\Omega > 2\sqrt{2}$ then the equality is attained and that the minimizers give rise to functions in $\mathrm{kr}(1/\lambda_\Omega + C_\sigma^m)$ and vice versa. We will not give these details in order to shorten the notes, see [3].

The constraint (5) needed in Theorem 1.5, appears precisely as a technical obstruction on the arguments that we use to prove that equality holds in (17). The items (*ii*) and (*iii*) in Theorem 2.2 ensure that

$$\lambda_\Omega = \sup\{|\lambda| : \mathrm{kr}(1/\lambda + C_\sigma^m) \neq 0\} \text{ and } 4/\lambda_\Omega = \inf\{|\lambda| : \mathrm{kr}(1/\lambda + C_\sigma^m) \neq 0\}. \tag{23}$$

2.3 *The Isoperimetric-Type Inequality*

Finally, in this subsection we gather the previous results and give the isoperimetric-type inequality in terms of area and capacity. Notice that we are looking for an inequality for λ_Ω.

At this point the following result become crucial. If Ω is a ball then $2W$ is an isometry and $\|W_\Omega\|_\sigma^2 = 1/4$. The opposite implication is proved in [5]. Thus, $\lambda_\Omega = 4\big(m\|K\|_\sigma + \sqrt{m^2\|K\|_\sigma^2 + 1/4}\big)$.

For a general Ω, $\|W\|_\sigma^2 \geq 1/4$ holds. Then,

$$\begin{aligned}\|K\|_\sigma &= \sup_{f \neq 0} \frac{1}{\|f\|_\sigma^2} \int Kf \cdot \overline{f} \geq \sigma(\partial\Omega) \iint \frac{1}{4\pi|x-y|} \frac{d\sigma(x)}{\sigma(\partial\Omega)} \frac{d\sigma(y)}{\sigma(\partial\Omega)} \\ &\geq \frac{\mathrm{Area}(\partial\Omega)}{\mathrm{Cap}(\Omega)}.\end{aligned}$$

Equality holds in the las two inequalities if Ω is a ball. Hence,

$$\lambda_\Omega \geq 4\left(m\,\frac{\mathrm{Area}(\partial\Omega)}{\mathrm{Cap}(\Omega)} + \sqrt{m^2\left(\frac{\mathrm{Area}(\partial\Omega)}{\mathrm{Cap}(\Omega)}\right)^2 + \frac{1}{4}}\right). \tag{24}$$

Therefore, combining (23) and (24) we get the desired result.

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Correlation Inequalities for Classical and Quantum XY Models

Costanza Benassi, Benjamin Lees, and Daniel Ueltschi

Abstract We review correlation inequalities of truncated functions for the classical and quantum XY models. A consequence is that the critical temperature of the XY model is necessarily smaller than that of the Ising model, in both the classical and quantum cases. We also discuss an explicit lower bound on the critical temperature of the quantum XY model.

Keywords Classical XY model • Correlation inequalities • Lattice systems • Quantum XY model • Spin systems

1 Setting and Results

The goal of this survey is to recall some results of old that have been rather neglected in recent years. We restrict ourselves to the cases of classical and quantum XY models. Correlation inequalities are an invaluable tool that allows to obtain the monotonicity of spontaneous magnetisation, the existence of infinite volume limits, and comparisons between the critical temperatures of various models. Many correlation inequalities have been established for the planar rotor (or classical XY) model, with interesting applications and consequences in the study of the phase diagram and the Gibbs states [1–7]. Some of these inequalities can also be proved for its quantum counterpart [8–11].

Let Λ be a finite set of sites. The classical XY model (or planar rotor model) is a model of interacting spins on such a lattice. The configuration space of the system is defined as $\Omega_\Lambda = \{\{\sigma_x\}_{x\in\Lambda} : \sigma_x \in \mathbb{S}^1 \;\forall x \in \Lambda\}$: each site hosts a unimodular vector lying on a unit circle. It is convenient to represent the spins by means of angles,

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A. Michelangeli, G. Dell'Antonio (eds.), *Advances in Quantum Mechanics*,
Springer INdAM Series 18, DOI 10.1007/978-3-319-58904-6_2

namely

$$\sigma_x^1 = \cos\phi_x \tag{1}$$

$$\sigma_x^2 = \sin\phi_x \tag{2}$$

with $\phi_x \in [0, 2\pi]$. The energy of a configuration $\sigma \in \Omega_\Lambda$ with angles $\phi = \{\phi_x\}_{x\in\Lambda}$ is

$$H_\Lambda^{\text{cl}}(\phi) = -\sum_{A\subset\Lambda} J_A^1 \prod_{x\in A} \sigma_x^1 + J_A^2 \prod_{x\in A} \sigma_x^2, \tag{3}$$

with $J_A^i \in \mathbb{R}$ for all $A \subset \Lambda$. The expectation value at inverse temperature β of a functional f on the configuration space is

$$\langle f\rangle_{\Lambda,\beta}^{\text{cl}} = \frac{1}{Z_{\Lambda,\beta}^{\text{cl}}} \int d\phi \mathrm{e}^{-\beta H_\Lambda^{\text{cl}}(\phi)} f(\phi), \tag{4}$$

where $Z_{\Lambda,\beta}^{\text{cl}} = \int d\phi \mathrm{e}^{-\beta H_\Lambda^{\text{cl}}(\phi)}$ is the partition function and $\int d\phi = \int_0^{2\pi} \dots \int_0^{2\pi} \prod_{x\in\Lambda} \frac{d\phi_x}{2\pi}$.

We now define the quantum XY model. We restrict ourselves to the spin-$\frac{1}{2}$ case. As before, the model is defined on a finite set of sites Λ; the Hilbert space is $\mathscr{H}_\Lambda^{\text{qu}} = \otimes_{x\in\Lambda}\mathbb{C}^2$. The spin operators acting on $\mathbb{C}^2$ are the three hermitian matrices S^i, $i = 1, 2, 3$, that satisfy $\left[S^1, S^2\right] = iS^3$ and its cyclic permutations, and $(S^1)^2 + (S^2)^2 + (S^3)^2 = \frac{3}{4}\mathbb{1}$. They are explicitly formulated in terms of Pauli matrices:

$$S^1 = \tfrac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S^2 = \tfrac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S^3 = \tfrac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5}$$

The hamiltonian describing the interaction is

$$H_\Lambda^{\text{qu}} = -\sum_{A\subset\Lambda} J_A^1 \prod_{x\in A} S_x^1 + J_A^2 \prod_{x\in A} S_A^2, \tag{6}$$

with $S_x^i = S^i \otimes \mathbb{1}_{\Lambda\setminus\{x\}}$. The $\{J_A^i\}_{A\subset\Lambda}$ are nonnegative coupling constants. The Gibbs state at inverse temperature β is

$$\langle \mathscr{O}\rangle_{\Lambda,\beta}^{\text{qu}} = \frac{1}{Z_{\Lambda,\beta}^{\text{qu}}} \operatorname{Tr} \mathscr{O}\, \mathrm{e}^{-\beta H_\Lambda^{\text{qu}}}, \tag{7}$$

with $Z_{\Lambda,\beta}^{\text{qu}} = \operatorname{Tr} \mathrm{e}^{-\beta H_\Lambda^{\text{qu}}}$ the partition function and $\mathscr{O}$ any operator acting on $\mathscr{H}_\Lambda^{\text{qu}}$.

The first result holds for both classical and quantum models.

Theorem 1.1 *Assume that $J^1_A, J^2_A \geq 0$ for all $A \subset \Lambda$. The following inequalities hold true for all $X, Y \subset \Lambda$, and for all $\beta > 0$.*

$$\text{Classical}: \quad \Big\langle \prod_{x\in X} \sigma^1_x \prod_{x\in Y} \sigma^1_x \Big\rangle^{\text{cl}}_{\Lambda,\beta} - \Big\langle \prod_{x\in X} \sigma^1_x \Big\rangle^{\text{cl}}_{\Lambda,\beta} \Big\langle \prod_{x\in Y} \sigma^1_x \Big\rangle^{\text{cl}}_{\Lambda,\beta} \geq 0,$$

$$\Big\langle \prod_{x\in X} \sigma^1_x \prod_{x\in Y} \sigma^2_x \Big\rangle^{\text{cl}}_{\Lambda,\beta} - \Big\langle \prod_{x\in X} \sigma^1_x \Big\rangle^{\text{cl}}_{\Lambda,\beta} \Big\langle \prod_{x\in Y} \sigma^2_x \Big\rangle^{\text{cl}}_{\Lambda,\beta} \leq 0.$$

$$\text{Quantum}: \quad \Big\langle \prod_{x\in X} S^1_x \prod_{x\in Y} S^1_x \Big\rangle^{\text{qu}}_{\Lambda,\beta} - \Big\langle \prod_{x\in X} S^1_x \Big\rangle^{\text{qu}}_{\Lambda,\beta} \Big\langle \prod_{x\in Y} S^1_x \Big\rangle^{\text{qu}}_{\Lambda,\beta} \geq 0,$$

$$\Big\langle \prod_{x\in X} S^1_x \prod_{x\in Y} S^2_x \Big\rangle^{\text{qu}}_{\Lambda,\beta} - \Big\langle \prod_{x\in X} S^1_x \Big\rangle^{\text{qu}}_{\Lambda,\beta} \Big\langle \prod_{x\in Y} S^2_x \Big\rangle^{\text{qu}}_{\Lambda,\beta} \leq 0.$$

In the quantum case, similar inequalities hold for Schwinger functions, see [11] for details. The proofs are given in Sects. 3 and 4 respectively. These inequalities are known as Ginibre inequalities—first introduced by Griffiths for the Ising model [12] and systematised in a seminal work by Ginibre [13], which provides a general framework for inequalities of this form. Ginibre inequalities for the classical XY model have then been established with different techniques [1, 3–5, 13]. The equivalent result for the quantum case has been proved with different approaches [8–11]. An extension to the ground state of quantum systems with spin 1 was proposed in [11]. A straightforward corollary of this theorem is monotonicity with respect to coupling constants, as we see now.

Corollary 1.2 *Assume that $J^1_A, J^2_A \geq 0$ for all $A \subset \Lambda$. Then for all $X, Y \subset \Lambda$, and for all $\beta > 0$*

$$\text{Classical}: \quad \frac{\partial}{\partial J^1_Y} \langle \prod_{x\in X} \sigma^1_x \rangle^{\text{cl}}_{\Lambda,\beta} \geq 0,$$

$$\frac{\partial}{\partial J^2_Y} \langle \prod_{x\in X} \sigma^1_x \rangle^{\text{cl}}_{\Lambda,\beta} \leq 0.$$

$$\text{Quantum}: \quad \frac{\partial}{\partial J^1_Y} \langle \prod_{x\in X} S^1_x \rangle^{\text{qu}}_{\Lambda,\beta} \geq 0,$$

$$\frac{\partial}{\partial J^2_Y} \langle \prod_{x\in X} S^1_x \rangle^{\text{qu}}_{\Lambda,\beta} \leq 0.$$

Interestingly this result appears to be not trivially true for the quantum Heisenberg ferromagnet. Indeed a toy version of the fully SU(2) invariant model has been provided explicitly, for which this result does not hold (nearest neighbours interaction on a three-sites chain with open boundary conditions) [14]. The question whether this result might still be established in a proper setting is still open. On the other hand, Ginibre inequalities have been proved for the classical Heisenberg ferromagnet [1, 2, 4].

Monotonicity of correlations with respect to temperature does not follow straightforwardly from the corollary. This can nonetheless be proved for the classical XY model.

Theorem 1.3 *Classical model: Assume that $J^1_A \geq |J^2_A|$ for all $A \subset \Lambda$, and that $J^2_A = 0$ whenever $|A|$ is odd. Then for all $A, B \subset \Lambda$, we have*

$$\frac{\partial}{\partial \beta}\Big\langle \prod_{x \in B} \sigma^1_x \Big\rangle^{\mathrm{cl}}_{\Lambda,\beta} \geq 0.$$

Let us restrict to the two-body case and assume that H^{cl}_Λ is given by

$$H^{\mathrm{cl}}_\Lambda = -\sum_{x,y \in \Lambda} J_{xy} \left(\sigma^1_x \sigma^1_y + \eta_{xy} \sigma^2_x \sigma^2_y\right).$$

Then if $|\eta_{xy}| \leq 1$ for all x, y,

$$\frac{\partial}{\partial J_{xy}} \langle \prod_{z \in A} \sigma^1_z \rangle^{\mathrm{cl}}_{\Lambda,\beta} \geq 0. \tag{8}$$

Notice that this theorem has a wider range of applicability than Corollary 1.2: in the theorem above, the coupling constants along one of the directions are allowed to be negative (though not too negative), while in the corollary the nonnegativity of all coupling constants a is necessary hypothesis. This result has been proposed and discussed in various works [4, 6, 13]—see Sect. 3 for the details. Unfortunately we lack a quantum equivalent of these statements.

We conclude this section by remarking that correlation inequalities in the quantum case can be applied also to other models of interest. For example, we consider a certain formulation of Kitaev's model (see [15] for its original formulation and [16] for a review of the topic). Let $\Lambda \subset\subset \mathbb{Z}^2$ be a square lattice with edges $\mathscr{E}_\Lambda$. Each *edge* of the lattice hosts a spin, i.e. the Hilbert space of this model is $\mathscr{H}^{\mathrm{Kitaev}}_\Lambda = \otimes_{e \in \mathscr{E}_\Lambda} \mathbb{C}^2$. The Kitaev hamiltonian is

$$H^{\mathrm{Kitaev}}_\Lambda = -\sum_{x \in \Lambda} J_x \prod_{\substack{e \in \mathscr{E}_\Lambda: \\ x \in e}} S^1_e + \sum_{F \subset \Lambda} J_F \prod_{e \subset F} S^3_e, \tag{9}$$

where F denotes the faces of the lattice, i.e. the unit squares which are the building blocks of $\mathbb{Z}^2$, J_x, J_F are ferromagnetic coupling constants and $S^i_e = S^i \otimes \mathbb{1}_{\mathscr{E}_\Lambda \setminus e}$. $H^{\mathrm{Kitaev}}_\Lambda$ has the same structure as hamiltonian (6) so Ginibre inequalities apply as well. It is not clear, though, whether this might lead to useful results for the study of this specific model.

Another relevant model is the *plaquette orbital model* that was studied in [17, 18]; interactions between neighbours x, y are of the form $-S_x^i S_y^i$, with i being equal to 1 or 3 depending on the edge.

2 Comparison Between Ising and XY Models

We now compare the correlations of the Ising and XY models and their respective critical temperatures. The configuration space of the Ising model is $\Omega_\Lambda^{\mathrm{Is}} = \{-1, 1\}^\Lambda$, that is, Ising configurations are given by $\{s_x\}_{x\in\Lambda}$ with $s_x = \pm 1$ for each $x \in \Lambda$. We consider many-body interactions, so the energy of a configuration $s \in \Omega_\Lambda^{\mathrm{Is}}$ is

$$H^{\mathrm{Is}}_{\Lambda,\{J_A\}}(s) = -\sum_{A\subset\Lambda} J_A \prod_{x\in A} s_x; \tag{10}$$

we assume that the system is "ferromagnetic", i.e. the coupling constants $J_A \geq 0$ are nonnegative. The Gibbs state at inverse temperature β is

$$\langle f\rangle^{\mathrm{Is}}_{\Lambda,\{J_A\},\beta} = \frac{1}{Z^{\mathrm{Is}}_{\Lambda,\{J_A\},\beta}} \sum_{s\in\Omega_\Lambda^{\mathrm{Is}}} f(s)\, \mathrm{e}^{-\beta H^{\mathrm{Is}}_{\Lambda,\{J_A\}}}, \tag{11}$$

with f any functional on $\Omega_\Lambda^{\mathrm{Is}}$ and $Z^{\mathrm{Is}}_{\Lambda,\{J_A\},\beta} = \sum_{s\in\Omega_\Lambda^{\mathrm{Is}}} \mathrm{e}^{-\beta H^{\mathrm{Is}}_{\Lambda,\{J_A\}}}$ is the partition function. The following result holds for both the classical [5] and the quantum case [9, 19].

Theorem 2.1 *Assume that $J_A^1, J_A^2 \geq 0$ for all $A \subset \Lambda$. Then for all $X \subset \Lambda$ and all $\beta > 0$,*

$$\textit{Classical:} \qquad \langle \prod_{x\in X} \sigma_x^1 \rangle^{\mathrm{cl}}_{\Lambda,\beta} \leq \langle \prod_{x\in X} s_x \rangle^{\mathrm{Is}}_{\Lambda,\{J_A^1\},\beta}.$$

$$\textit{Quantum:} \qquad \langle \prod_{x\in X} S_x^1 \rangle^{\mathrm{qu}}_{\Lambda,\beta} \leq 2^{-|X|} \langle \prod_{x\in X} s_x \rangle^{\mathrm{Is}}_{\Lambda,\{J_A^*\},\beta},$$

with $J_A^* = 2^{-|A|} J_A^1$.

A review of the proof of the classical case is proposed in Sect. 3. In the quantum case, this statement for spin-$\frac{1}{2}$ is a straightforward consequence of Corollary 1.2, but interestingly this result has been extended to any value of the spin [19]. We review the proof of this general case in Sect. 4.

We now consider the case of spin-$\frac{1}{2}$ and pair interactions, that is, the hamiltonian is

$$H_\Lambda^{\rm qu} = -\sum_{x,y \in \Lambda} (S_x^1 S_y^1 + S_x^2 S_y^2). \tag{12}$$

We define the *spontaneous magnetisation* $m(\beta)$ at inverse temperature β by

$$m(\beta)^2 = \liminf_{\Lambda \nearrow \mathbb{Z}^d} \frac{1}{|\Lambda|^2} \sum_{x,y \in \Lambda} \langle S_x^1 S_y^1 \rangle_{\Lambda,\beta}^{\rm qu}. \tag{13}$$

We define the critical temperature for the model $T_{\rm c}^{\rm qu} = 1/\beta_{\rm c}^{\rm qu}$ as

$$\beta_{\rm c}^{\rm qu} = \sup\{\beta > 0 : m(\beta) = 0\}, \tag{14}$$

where $\beta_{\rm c}^{\rm qu} \in (0, \infty]$. A consequence of Theorem 2.1 is the following.

Corollary 2.2 *The critical temperatures satisfy*

$$T_{\rm c}^{\rm qu} \leq \tfrac{1}{4} T_{\rm c}^{\rm Ising}.$$

The critical temperature of the Ising model in the three-dimensional cubic lattice has been calculated numerically and is $T_{\rm c}^{\rm Ising} = 4.511 \pm 0.001$ [20]. It is $T_{\rm c}^{\rm cl} = 2.202 \pm 0.001$ [21] for the classical model and $T_{\rm c}^{\rm qu} = 1.008 \pm 0.001$ for the quantum model (S. Wessel, private communication).

A major result of mathematical physics is the rigorous proof of the occurrence of long-range order in the classical and quantum XY models, in dimensions three and higher, and if the temperature is low enough [22, 23]. The method can be used to provide a rigorous lower bound on critical temperatures; the following theorem concerns the quantum model.

Theorem 2.3 *For the three-dimensional cubic lattice, the temperature of the quantum XY model satisfies*

$$T_{\rm c}^{\rm qu} \geq 0.323.$$

The best rigorous upper bound on the critical temperature of the three-dimensional Ising model is $T_c^{\rm Ising} \leq 5.0010$ [24]. Together with the above corollary and theorem, we get

$$0.323 \leq T_{\rm c}^{\rm qu} \leq \tfrac{1}{4} T_{\rm c}^{\rm Ising} \leq 1.250. \tag{15}$$

Proof (Theorem 2.3) We consider the XY model with spins in the 1–3 directions for convenience. We make use of the result [25, Theorem 5.1], that was obtained with the method of reflection positivity and infrared bounds [22, 23]. Precisely, we use Eqs. (5.54), (5.57) and (5.63) of [25].

$$m(\beta)^2 \geq \begin{cases} \frac{1}{4} - \frac{J_3}{2}\sqrt{\langle S_0^1 S_{e_1}^1 \rangle^{\mathrm{qu}}} - \frac{K_3}{\beta} \\ \langle S_0^1 S_{e_1}^1 \rangle_\Lambda^{\mathrm{qu}} - \frac{I_3}{2}\sqrt{\langle S_0^1 S_{e_1}^1 \rangle^{\mathrm{qu}}} - \frac{K_3'}{\beta} \end{cases} \tag{16}$$

where e_1 is a nearest neighbour of the origin, and J_3, I_3, K_3, K_3' are real numbers coming from explicit integrals. Their values are $J_3 = 1.15672$; $I_3 = 0.349884$; $K_3 = 0.252731$; and $K_3' = 0.105107$. Notice that β is rescaled by a factor 2 with respect to [25], due to a different choice of coupling constants in the hamiltonian. Let $x = \sqrt{\langle S_0^1 S_{e_1}^1 \rangle^{\mathrm{qu}}}$; since we do not have good bounds on x, we treat it as an unknown. The magnetisation $m(\beta)$ is guaranteed to be positive if $x \leq t$ where t is the zero of $\frac{1}{4} - \frac{K_3}{\beta} - \frac{J_3}{2}x$; or $x \geq r_+$, where r_+ is the largest zero of $x^2 - \frac{I_3}{2}x - \frac{K_3'}{\beta}$. At least one of these holds true when $r_+ < t$, that is, when

$$\frac{1}{2}\left(\frac{I_3}{2} + \sqrt{\frac{I_3^2}{4} + \frac{4K_3'}{\beta}}\right) < \frac{1}{2J_3} - \frac{1}{\beta}\frac{2K_3}{J_3} \tag{17}$$

This is the case for $1/\beta < 0.323$ giving the upper bound $T_c \geq 0.323$.

3 Proofs for the Classical XY Model

The proofs require several steps and additional lemmas. The following paragraphs are devoted to a complete study of their proofs. Given local variables $\{\sigma_x\}_{x\in\Lambda}$, we denote $\sigma_A^i = \prod_{x\in A}\sigma_x^i$ for $A \subset \Lambda$.

3.1 Griffiths and FKG Inequalities, and Proof of Theorem 1.1

We start with Theorem 1.1. We describe the approach proposed in [1, 5], and use a similar notation. Their framework relies on some well known properties of the Ising model and on the so called FKG inequality.

Lemma 3.1 (Griffiths Inequalities for the Ising Model) *Let f and g be functionals on $\Omega_\Lambda^{\mathrm{Is}}$ such that they can be expressed as power series of $\prod_{x\in A} s_x$, $A \subset \Lambda$ with positive coefficients. Then*

$$\langle f \rangle^{\mathrm{Is}}_{\Lambda,\{J_A\},\beta} \geq 0;$$

$$\langle fg \rangle^{\mathrm{Is}}_{\Lambda,\{J_A\},\beta} \geq \langle f \rangle^{\mathrm{Is}}_{\Lambda,\{J_A\},\beta}\langle g \rangle^{\mathrm{Is}}_{\Lambda,\{J_A\},\beta}.$$

We do not provide the proof of this result—see [12, 13] for the original formulation and [26] for a modern description. An immediate consequence is the following.

Corollary 3.2 *Given f with the properties in Lemma 3.1, we have for any $A \subset \Lambda$*

$$\frac{\partial}{\partial J_A} \langle f \rangle^{\mathrm{Is}}_{\Lambda,\{J_A\},\beta} \geq 0.$$

Another result which is very useful in this framework is the so called FKG inequality. We formulate it in a specific setting. Let $\mathscr{I}_N = \left[0, \frac{\pi}{2}\right]^N$ for some $N \in \mathbb{N}$. Any $\psi \in \mathscr{I}_N$ is then a collection of angles $\psi = (\psi_1, \ldots, \psi_N)$. It is possible to introduce a partial ordering relation on $\mathscr{I}_N$ as follows: for any $\psi, \xi \in \mathscr{I}_N$, $\psi \leq \xi$ if and only if $\psi_i \leq \xi_i$ for all $i \in \{1, \ldots, N\}$. A function f on $\mathscr{I}_N$ is said to be increasing (or decreasing) if $\psi \leq \xi$ implies $f(\psi) \leq f(\xi)$ (or $f(\psi) \geq f(\xi)$) for all $\psi, \xi \in \mathscr{I}_N$. The following result holds.

Lemma 3.3 (FKG Inequality) *Let $d\nu(\psi) = p(\psi) \prod_{i=1}^N d\mu(\psi_i)$ be a normalised measure on $\mathscr{I}_N$, with $d\mu(\psi_i)$ a normalised measure on $\left[0, \frac{\pi}{2}\right]$, $p(\psi) \geq 0$ for all $\psi \in \mathscr{I}_N$ and*

$$p(\psi \vee \xi) p(\psi \wedge \xi) \geq p(\psi) p(\xi), \tag{18}$$

where $(\psi \vee \xi)_i = \max(\psi_i, \xi_i)$ and $(\psi \wedge \xi)_i = \min(\psi_i, \xi_i)$. Then for any f and g increasing (or decreasing) functions on $\mathscr{I}_N$

$$\int fg d\nu \geq \int f d\nu \int g d\nu.$$

The inequality changes sign if one of the functions is increasing and the other is decreasing.

We also skip the proof of this statement. We refer to [27] for the original result, to [5, 28] for the formulation above, and [26] for its relevance in the study of the Ising model.

Before turning to the actual proof of the theorem, we introduce another useful lemma.

Lemma 3.4 *Let $\{q_x\}_{x \in \Lambda}$ be a collection of positive increasing (decreasing) functions on $\left[0, \frac{\pi}{2}\right]$. Then for any $\theta, \psi \in \mathscr{I}_{|\Lambda|}$ and any $A \subset \Lambda$,*

$$q_A(\theta \vee \psi) + q_A(\theta \wedge \psi) \geq q_A(\psi) + q_A(\theta).$$

We do not provide the proof here, see [5, 28] for more details. We can now discuss the proof of Theorem 1.1.

Proof (Theorem 1.1) Since the temperature does not play any rôle in this section, we set $\beta = 1$ in the following and we drop any dependency on it. The main idea of the proof is to describe a classical XY spin as a pair of Ising spins and an angular variable. The new notation for $\sigma_x \in \mathbb{S}^1$ is

$$\sigma_x^1 = \cos(\theta_x) U_x, \tag{19}$$

$$\sigma_x^2 = \sin(\theta_x) V_x, \tag{20}$$

with $U_x, V_x \in \{-1, 1\}$ for all $x \in \Lambda$ and $\theta = (\theta_{x_1}, \ldots, \theta_{x_\Lambda}) \in \mathscr{I}_{|\Lambda|}$. With this notation, it is possible to express H_Λ^{cl} of Eq. (3) as the sum of two Ising hamiltonians with spins $\{U_x\}_{x\in\Lambda}$, $\{V_x\}_{x\in\Lambda}$ respectively:

$$H_\Lambda^{\mathrm{cl}}(\theta, U, V) = -\sum_{A\subset\Lambda} \left(J_A^1 \prod_{x\in A} \cos(\theta_x) U_A + J_A^2 \prod_{x\in A} \sin(\theta_x) V_A \right) \tag{21}$$

$$= H^{\mathrm{Is}}_{\Lambda,\{\cos(\theta)_A J_A^1\}}(U) + H^{\mathrm{Is}}_{\Lambda,\{\sin(\theta)_A J_A^2\}}(V). \tag{22}$$

Let us introduce the notation: $J_A^1 \prod_{x\in A} \cos(\theta_x) = \mathcal{J}_A(\theta)$, $J_A^2 \prod_{x\in A} \sin(\theta_x) = \mathcal{K}_A(\theta)$, $\int d\theta = \int_0^{\frac{\pi}{2}} \ldots \int_0^{\frac{\pi}{2}} \prod_{x\in\Lambda} \frac{2}{\pi} d\theta_x$. Then

$$\langle \sigma_X^1 \sigma_Y^1 \rangle_{H_\Lambda^{\mathrm{cl}}} = \frac{\int d\theta\, Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{J}_A(\theta)\}} Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta)\}} \cos(\theta)_X \cos(\theta)_Y \langle U_X U_Y \rangle^{\mathrm{Is}}_{\Lambda,\{\mathcal{J}_A(\theta)\}}}{\int d\theta\, Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{J}_A(\theta)\}} Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta)\}}}$$

$$\geq \frac{\int d\theta\, Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{J}_A(\theta)\}} Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta)\}} \cos(\theta)_X \langle U_X \rangle^{\mathrm{Is}}_{\Lambda,\{\mathcal{J}_A(\theta)\}} \cos(\theta)_Y \langle U_Y \rangle^{\mathrm{Is}}_{\Lambda,\{\mathcal{J}_A(\theta)\}}}{\int d\theta\, Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{J}_A(\theta)\}} Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta)\}}}.$$

The inequality above follows from Lemma 3.1. Moreover

$$\langle \sigma_X^1 \sigma_Y^2 \rangle_{H_\Lambda^{\mathrm{cl}}} = \frac{\int d\theta Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{J}_A(\theta)\}} Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta)\}} \cos(\theta)_X \langle U_X \rangle^{\mathrm{Is}}_{\Lambda,\{\mathcal{J}_A(\theta)\}} \sin(\theta)_Y \langle V_Y \rangle^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta)\}}}{\int d\theta\, Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{J}_A(\theta)\}} Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta)\}}}.$$

$\cos(\theta)_X$ and $\sin(\theta)_X$ are respectively decreasing and increasing on $\mathscr{I}_{|\Lambda|}$ for any $X \subset \Lambda$. Let us now consider $\langle U_X \rangle^{\mathrm{Is}}_{\Lambda,\{\mathcal{J}_A(\theta)\}}$. By Corollary 3.2, it is a decreasing function on $\mathscr{I}_{|\Lambda|}$ for any $X \subset \Lambda$, since the coupling constants of $H^I_{\Lambda,\{\mathcal{J}_A(\theta)\}}$ are decreasing in θ. Analogously, $\langle V_X \rangle^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta)\}}$ is an increasing function on $\mathscr{I}_{|\Lambda|}$ for any $X \subset \Lambda$. Theorem 1.1 is then a simple consequence of Lemma 3.3, with $d\mu(\theta_x) = \frac{2}{\pi} d\theta_x$ and

$$p(\theta) = \frac{Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{J}_A(\theta)\}} Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta)\}}}{\int d\theta\, Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{J}_A(\theta)\}} Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta)\}}}. \tag{23}$$

The last step missing is to show that $p(\theta)$ defined as above fulfills hypothesis (18) of Lemma 3.3. This amounts to showing

$$Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta\vee\psi)\}} Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta\wedge\psi)\}} \geq Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta)\}} Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\psi)\}}; \tag{24}$$

$$Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{J}_A(\theta\vee\psi)\}} Z^{\mathrm{I}}_{\Lambda,\{\mathcal{J}_A(\theta\wedge\psi)\}} \geq Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{J}_A(\theta)\}} Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{J}_A(\psi)\}}. \tag{25}$$

Since the arguments to prove these inequalities are very similar, we prove explicitly only the first one. Equation (24) is equivalent to

$$\left(\frac{Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta)\}}}{Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta\wedge\psi)\}}}\right)^{-1} \left(\frac{Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta\vee\psi)\}}}{Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\psi)\}}}\right) \geq 1 \tag{26}$$

Notice that

$$\left(\frac{Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta)\}}}{Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta\wedge\psi)\}}}\right)^{-1} \left(\frac{Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta\vee\psi)\}}}{Z^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\psi)\}}}\right) = \frac{\left\langle \mathrm{e}^{-H^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta\vee\psi)-\mathcal{K}_A(\psi)\}}} \right\rangle^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\psi)\}}}{\left\langle \mathrm{e}^{-H^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta)-\mathcal{K}_A(\theta\wedge\psi)\}}} \right\rangle^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta\wedge\psi)\}}}.$$

Thanks to Lemma 3.4, the functions whose expectation value we are computing above fulfill the hypothesis of Lemma 3.1 and Corollary 3.2. Then, applying Lemma 3.4 and Corollary 3.2,

$$\begin{aligned} \left\langle \mathrm{e}^{-H^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta\vee\psi)-\mathcal{K}_A(\psi)\}}} \right\rangle^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\psi)\}} &\geq \left\langle \mathrm{e}^{-H^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta)-\mathcal{K}_A(\theta\wedge\psi)\}}} \right\rangle^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\psi)\}} \\ &\geq \left\langle \mathrm{e}^{-H^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta)-\mathcal{K}_A(\theta\wedge\psi)\}}} \right\rangle^{\mathrm{Is}}_{\Lambda,\{\mathcal{K}_A(\theta\wedge\psi)\}}. \end{aligned} \tag{27}$$

Hence $p(\theta)$ has the required property.

3.2 Proof of Theorem 1.3

Let us now turn to Theorem 1.3. We follow the framework described in [4, 13].

Lemma 3.5 *Let H^{cl}_Λ be the hamiltonian defined in (3). If $J^1_A \geq |J^2_A|$ for all $A \subset \Lambda$ and $J^2_A = 0$ for $|A|$ odd, then there exist non negative coupling constants $\{K_M\}_{M\in\mathbb{Z}^\Lambda}$ such that*

$$H^{\mathrm{cl}}_\Lambda(\phi) = -\sum_{M\in\mathbb{Z}^\Lambda} K_M \cos\left(M\cdot\phi\right), \tag{28}$$

where, given $M \in \mathbb{Z}^\Lambda$, $M = (m_1, m_2, \ldots, m_\Lambda)$, $M\cdot\phi = \sum_{x\in\Lambda} m_x\phi_x$.

Proof The statement follows from the two following identities:

$$\cos(\theta)\cos(\chi) = \frac{1}{2}(\cos(\theta-\chi)+\cos(\theta+\chi)), \tag{29}$$

$$\sin(\theta)\sin(\chi) = \frac{1}{2}(\cos(\theta-\chi)-\cos(\theta+\chi)), \tag{30}$$

$\forall\theta,\chi\in[0,2\pi]$.

A necessary step for this lemma and for Theorem 1.3 is duplication of variables [13]: we consider two sets of angles (i.e. spins) on the lattice instead of just one, and denote them by $\{\phi_x\}_{x\in\Lambda}$ and $\{\bar{\phi}_x\}_{x\in\Lambda}$. The hamiltonian for the $\{\bar{\phi}_x\}$ is

$$\begin{aligned}\bar{H}^{\mathrm{cl}}_\Lambda(\bar{\phi}) &= -\sum_{A\subset\Lambda}\left(\bar{J}^1_A\bar{\sigma}^1_A+\bar{J}^2_A\bar{\sigma}^2_A\right)\\ &= -\sum_{M\in\mathbb{Z}^\Lambda}\bar{K}_M\cos(M\cdot\bar{\phi}).\end{aligned} \tag{31}$$

Here, $\{\bar{\sigma}_x\}$ are related to $\{\bar{\phi}_x\}$ as in Eqs. (1) and (2). The $\bar{J}^i_A$ are non negative coupling constants with $\bar{J}^1_A \geq |\bar{J}^2_A| \geq 0$ and $\{\bar{K}_M\}$ are as in Lemma 3.5. A composite hamiltonian can be defined as

$$\begin{aligned}&-\hat{H}_\Lambda(\phi,\bar{\phi}) = -H^{\mathrm{cl}}_\Lambda(\phi)-\bar{H}^{\mathrm{cl}}_\Lambda(\bar{\phi})\\ &= \sum_{M\in\mathscr{M}}\tfrac{K_M+\bar{K}_M}{2}\left(\cos(M\cdot\phi)+\cos(M\cdot\bar{\phi})\right)+\tfrac{K_M-\bar{K}_M}{2}\left(\cos(M\cdot\phi)-\cos(M\cdot\bar{\phi})\right)\end{aligned} \tag{32}$$

In the following we always suppose $K_M \geq \bar{K}_M$ for all $M\in\mathbb{Z}^\Lambda$.The expectation value of any functional $f(\phi,\bar{\phi})$ can be written as

$$\langle f\rangle_{\hat{H}_\Lambda,\beta} = \frac{1}{Z_{H_\Lambda,\beta}Z_{\bar{H}_\Lambda,\beta}}\int d\phi d\bar{\phi}\mathrm{e}^{-\beta\hat{H}_\Lambda(\phi,\bar{\phi})}f(\phi,\bar{\phi}). \tag{33}$$

Lemma 3.6 *Suppose $f(\phi,\bar{\phi})$ belongs to the cone generated by* $\cos(M\cdot\phi)\pm\cos(M\cdot\bar{\phi})$*, $M\in\mathbb{Z}^\Lambda$, i.e. f can be written as product, sum or multiplication by a positive scalar of objects of that form. Then*

$$\langle f\rangle_{\hat{H}_\Lambda,\beta}\geq 0. \tag{34}$$

Proof Firstly, notice that

$$\int d\phi d\bar{\phi}\prod_{s=1}^{n}(\cos(M_s\cdot\phi)\pm\cos(M_s\cdot\bar{\phi})\geq 0 \tag{35}$$

for any $M_1, \dots, M_n \in \mathbb{Z}^\Lambda$ and any sequence of $(\pm)$. This follows from

$$\cos(M \cdot \phi) + \cos(M \cdot \bar{\phi}) = 2\cos(M \cdot \Phi)\cos(M \cdot \bar{\Phi}), \tag{36}$$

$$\cos(M \cdot \phi) - \cos(M \cdot \bar{\phi}) = 2\sin(M \cdot \Phi)\sin(M \cdot \bar{\Phi}), \tag{37}$$

with $\Phi_i = \frac{1}{2}(\phi_i + \bar{\phi}_i)$ and $\bar{\Phi}_i = \frac{1}{2}(\phi_i - \bar{\phi}_i)$. The integral (35) can be formulated as

$$\int d\Phi d\bar{\Phi} F(\Phi) F(\bar{\Phi}) = \left(\int d\Phi F(\Phi) \right)^2 \geq 0, \tag{38}$$

with $F(\Phi)$ an appropriate product of sines, cosines and positive constants.

Let us now turn to $\langle f \rangle_{\hat{H}_\Lambda,\beta}$. Since the partition function is always positive, we can focus on

$$\int d\phi d\bar{\phi} \mathrm{e}^{-\beta \hat{H}_\Lambda(\phi,\bar{\phi})} f(\phi, \bar{\phi}). \tag{39}$$

By a Taylor expansion of $\mathrm{e}^{-\beta \hat{H}_\Lambda(\phi,\bar{\phi})}$ and by the properties of f, this can be expressed as a sum with positive coefficients of integrals in the form (35). Hence the nonnegativity of the expectation value.
We have now all we need to prove Theorem 1.3.

Proof (Theorem 1.3) In order to prove the first statement of the theorem we use the formulation of the hamiltonian described in Lemma 3.5. Moreover, since σ_A^1 can be clearly expressed as the sum (with positive coefficients) of terms of the form $\cos(M \cdot \phi)$, $M \in \mathbb{Z}^\Lambda$, it is enough to prove that for any $M, N \in \mathbb{Z}^\Lambda$

$$\begin{aligned} &\frac{\partial}{\partial K_N} \langle \cos(M \cdot \phi) \rangle^{\mathrm{cl}}_{\Lambda,\beta} \\ &= \langle \cos(M \cdot \phi)\cos(N \cdot \phi) \rangle^{\mathrm{cl}}_{\Lambda,\beta} - \langle \cos(M \cdot \phi) \rangle^{\mathrm{cl}}_{\Lambda,\beta} \langle \cos(N \cdot \phi) \rangle^{\mathrm{cl}}_{\Lambda,\beta} \geq 0. \end{aligned} \tag{40}$$

Consider now the hamiltonian $\hat{H}_\Lambda$ introduced above and $\langle \cdot \rangle_{\hat{H}_\Lambda,\beta}$ the corresponding Gibbs state. From Lemma 3.6 we have

$$\langle \left(\cos(M \cdot \phi) - \cos(M \cdot \bar{\phi}) \right) \left(\cos(N \cdot \phi) - \cos(N \cdot \bar{\phi}) \right) \rangle_{\hat{H}_\Lambda,\beta} \geq 0. \tag{41}$$

If we take the limit $\bar{K}_M \nearrow K_M$, we find twice the expression in Eq. (40). Hence the result.

Let us now turn to the second statement of the theorem. In the case of two-body interaction H^{cl}_Λ assumes the form (8), which, with a notation resembling the one introduced in Lemma 3.5 can be explicitly formulated as

$$H^{\mathrm{cl}}_\Lambda(\phi) = -\sum_{x,y \in \Lambda} K^-_{xy} \cos(\phi_x - \phi_y) + K^+_{xy} \cos(\phi_x + \phi_y) \tag{42}$$

with

$$K_{xy}^{\pm} = \frac{J_{xy}}{2}\left(1 \mp \eta_{xy}\right). \tag{43}$$

Clearly $K_{xy}^{\pm}$ is analogous to the K_M introduced in Lemma 3.5 for $M \in \mathbb{Z}^{\Lambda}$ such that all its elements are zero except $m_x = 1,\ m_y = \pm 1$. Then we have

$$\frac{\partial}{\partial J_{xy}}\langle \sigma_A \rangle_{H_\Lambda^{\rm cl}} = \frac{1+\eta_{xy}}{2}\frac{\partial}{\partial K_{xy}^{-}}\langle \sigma_A \rangle_{H_\Lambda^{\rm cl}} + \frac{1-\eta_{xy}}{2}\frac{\partial}{\partial K_{xy}^{+}}\langle \sigma_A \rangle_{H_\Lambda^{\rm cl}}. \tag{44}$$

Due to Eq. (40) the expression above is the sum of two positive terms, hence it is positive.

3.3 *Proof of Theorem 2.1*

In this section we discuss the proof of Theorem 2.1 for the classical XY model. We use some of the concepts introduced in Sect. 3.2. The present proof has been proposed in [1, 5].

Proof (Theorem 2.1) As for the proof of Theorem 1.1, we express the XY spins by means of two Ising spins and an angle in $\left[0, \frac{\pi}{2}\right]$—see Eqs. (19) and (20) for the explicit expression of the spins and (22) for the new formulation of the hamiltonian $H_\Lambda^{\rm cl}$. With the same notation:

$$\begin{aligned}
\langle \sigma_X^1 \rangle_{H_\Lambda^{\rm cl}} &= \frac{\int d\theta\, Z^{\rm Is}_{\Lambda,\{\mathcal{J}_A(\theta)\}} Z^{\rm Is}_{\Lambda,\{\mathcal{K}_A(\theta)\}} \cos(\theta)_X \langle U_X \rangle^{\rm Is}_{\Lambda,\{\mathcal{J}_A(\theta)\}}}{\int d\theta\, Z^{\rm Is}_{\Lambda,\{\mathcal{J}_A(\theta)\}} Z^{\rm Is}_{\Lambda,\{\mathcal{K}_A(\theta)\}}} \\
&\leq \frac{\int d\theta\, Z^{\rm Is}_{\Lambda,\{\mathcal{J}_A(\theta)\}} Z^{\rm Is}_{\Lambda,\{\mathcal{K}_A(\theta)\}} \max_{\theta \in \mathscr{I}_{|\Lambda|}} \langle U_X \rangle^{\rm Is}_{\Lambda,\{\mathcal{J}_A(\theta)\}}}{\int d\theta\, Z^{\rm Is}_{\Lambda,\{\mathcal{J}_A(\theta)\}} Z^{\rm Is}_{\Lambda,\{\mathcal{K}_A(\theta)\}}} \\
&= \langle U_A \rangle^{\rm Is}_{\Lambda,\{J_A^1\}}.
\end{aligned} \tag{45}$$

4 Proof for the Quantum XY Model

We now discuss the proof of Theorem 1.1 in the quantum case. This theorem has been proved for pair interaction in [8], and it has been proposed independently in various works for more generic interactions [9–11]. We describe here the simpler approach proposed in [11]. Since the temperature does not play any role from now on, we set $\beta = 1$ and omit any dependency on it in the following. As for the classical case we introduce the notation $S_A^i = \prod_{x \in A} S_x^i$.

Proof (Theorem 1.1) For the proof it is convenient to perform a unitary transformation on the hamiltonian (6) and consider its version with interactions along the first and third directions of spin, namely

$$H_\Lambda^{\mathrm{qu}} = -\sum_{A\subset\Lambda} J_A^1 S_A^1 + J_A^3 S_A^3, \tag{46}$$

with $J_A^3 = J_A^2$ for all $A \subset \Lambda$.

The proof of this theorem uses some techniques similar to the ones introduced for the classical Theorem 1.3. These were indeed introduced by Ginibre [13] in a general framework. As for the classical case, it is convenient to duplicate the model. We introduce a new doubled Hilbert space $\bar{\mathscr{H}}_\Lambda = \mathscr{H}_\Lambda \otimes \mathscr{H}_\Lambda$. Given an operator $\mathscr{O}$ acting on $\mathscr{H}_\Lambda$ we define two operators acting on $\bar{\mathscr{H}}_\Lambda$,

$$\mathscr{O}_\pm = \mathscr{O} \otimes \mathbb{1} \pm \mathbb{1} \otimes \mathscr{O}. \tag{47}$$

The hamiltonian we consider for the doubled system is $H_{\Lambda,+}^{\mathrm{qu}}$:

$$H_{\Lambda,+}^{\mathrm{qu}} = H_\Lambda^{\mathrm{qu}} \otimes \mathbb{1}_\Lambda + \mathbb{1}_\Lambda \otimes H_\Lambda^{\mathrm{qu}} = -\sum_{A\subset\Lambda} J_A^1 (S_A^1)_+ + J_A^3 (S_A^3)_+ \tag{48}$$

The Gibbs state is denoted as

$$\langle\langle O \rangle\rangle = \frac{1}{(Z_\Lambda^{\mathrm{qu}})^2} \mathrm{Tr}\, O\, \mathrm{e}^{-H_{\Lambda,+}^{\mathrm{qu}}}, \tag{49}$$

for any operator O acting on $\bar{\mathscr{H}}_\Lambda$. It follows from some straightforward algebra that

$$\langle \mathscr{O}\mathscr{P} \rangle_\Lambda^{\mathrm{qu}} - \langle \mathscr{O} \rangle_\Lambda^{\mathrm{qu}} \langle \mathscr{P} \rangle_\Lambda^{\mathrm{qu}} = \frac{1}{2} \langle\langle \mathscr{O}_- \mathscr{P}_- \rangle\rangle; \tag{50}$$

$$(\mathscr{O}\mathscr{P})_\pm = \frac{1}{2} \left(\mathscr{O}_+ \mathscr{P}_\pm + \mathscr{O}_- \mathscr{P}_\mp \right), \tag{51}$$

for any $\mathscr{O}$, $\mathscr{P}$ operators on $\mathscr{H}_\Lambda$.

Just as $\mathbb{C}^2$ constitutes the "building block" for $\mathscr{H}_\Lambda$, so $\mathbb{C}^2 \otimes \mathbb{C}^2$ is to $\bar{\mathscr{H}}_\Lambda$. We can provide an explicit basis of $\mathbb{C}^2 \otimes \mathbb{C}^2$ such that S_+^1, S_-^1, S_+^3, $-S_-^3$ have all non negative elements:

$$|\mu_+\rangle = \frac{1}{\sqrt{2}} \left(|++\rangle + |--\rangle \right), \qquad |\mu_-\rangle = \frac{1}{\sqrt{2}} \left(|++\rangle - |--\rangle \right), \tag{52}$$

$$|\nu_+\rangle = \frac{1}{\sqrt{2}} \left(|+-\rangle + |-+\rangle \right), \qquad |\nu_-\rangle = \frac{1}{\sqrt{2}} \left(|+-\rangle - |-+\rangle \right). \tag{53}$$

Above by $|+\rangle$ and $|-\rangle$ we denote the basis of $\mathbb{C}^2$ formed by eigenvectors of S^3 with eigenvalues $\frac{1}{2}$ and $-\frac{1}{2}$ respectively, and $|i,j\rangle = |i\rangle \otimes |j\rangle$. It can be easily checked that the basis above has the required property. This result implies straightforwardly that there exists a basis of $\bar{\mathscr{H}}_\Lambda$ such that $(S^1_x)_+$, $(S^1_x)_-$, $(S^3_x)_+$ and $(-S^3_x)_-$ have non negative element for all $x \in \Lambda$. Let us consider the truncated correlation function we are interested in:

$$\left\langle \prod_{x\in X} S^1_x \prod_{x\in Y} S^1_x \right\rangle^{\text{qu}}_\Lambda - \left\langle \prod_{x\in X} S^1_x \right\rangle^{\text{qu}}_\Lambda \left\langle \prod_{x\in Y} S^1_x \right\rangle^{\text{qu}}_\Lambda = \tfrac{1}{2}\langle\langle \left(S^1_X\right)_- \left(S^1_Y\right)_- \rangle\rangle. \tag{54}$$

We can evaluate the right hand side of the equation above by a Taylor expansion:

$$(Z^{\text{qu}}_\Lambda)^2 \langle\langle \left(S^1_X\right)_- \left(S^1_Y\right)_- \rangle\rangle = \sum_{n\geq 0} \frac{1}{n!} \text{Tr} \left(S^1_X\right)_- \left(S^1_Y\right)_- (-H^{\text{qu}}_{\Lambda,+})^n \tag{55}$$

Given the formulation of $H^{\text{qu}}_{\Lambda,+}$ as in Eq. (48) and relation (51), it is clear that it can be expressed as a polynomial with positive coefficients of operators with nonnegative elements. The same holds for $(S^1_X)_-$ and$(S^1_Y)_-$. The trace of operators with nonnegative elements is non negative, hence the first inequality of the theorem. The second inequality can be proved precisely in the same way (with S^2_Y substituted by S^3_Y), by noticing that $(S^3_Y)_-$ has necessarily non positive elements.

Let us now turn to Theorem 2.1. While in the classical case it is necessary to introduce an artificial framework, interestingly the proof for the quantum case does not require such a construction. For spin-$\frac{1}{2}$ the statement can be easily recovered by recalling that the *classical* Ising model can be recovered as a particular case of the *quantum* XY model (not of the classical one!). We review here a more general proof valid for any value of spin $\mathscr{S}$ [19].

Proof (Theorem 2.1) We reformulate the quantum Hamiltonian in order to have the interaction along the first and the third axis, as in Eq. (46). We prove here the following result, which is unitarily equivalent to the statement of the theorem:

$$\left\langle S^3_X \right\rangle^{\text{qu}}_{\Lambda,\beta} \leq \mathscr{S}^{|X|} \langle s_A \rangle^{\text{Is}}_{\Lambda,\{\mathscr{S}^{|A|} J^3_A\},\beta}. \tag{56}$$

From now on we set $\beta = 1$ and drop all the dependencies on β since it does not play any role. Let $\mathcal{S}^i_x = \mathscr{S}^{-1} S^i_x$ be the rescaled spin operators. The models we compare are the following:

$$H^{\text{qu}}_{\Lambda,\mathcal{S}} = -\sum_{A\subset\Lambda} J^1_A \mathcal{S}^1_A + J^3_A \mathcal{S}^3_A, \tag{57}$$

$$H^{\text{Is}}_{\Lambda,\{J^3_A\}} = -\sum_{A\subset\Lambda} J^3_A s_A. \tag{58}$$

Clearly, (56) is equivalent to

$$\langle \mathcal{S}_X^3 \rangle_{\Lambda,\mathcal{S}}^{\mathrm{qu}} \leq \langle s_X \rangle_{\Lambda,\{J_A^3\}}^{\mathrm{Is}}. \tag{59}$$

This is what we aim to prove. Let us now build a composite system where each site of the lattice hosts a quantum degree of freedom and an Ising variable at the same time. Let $\mathscr{H} = H_{\Lambda,\mathcal{S}}^{\mathrm{qu}} + H_{\Lambda,\{J_A^3\}}^{\mathrm{Is}}$, i.e.

$$\mathscr{H} = -\sum_{A\subset\Lambda} J_A^1 \mathcal{S}_A^1 + J_A^3 (s_A + \mathcal{S}_A^3). \tag{60}$$

The Gibbs state is the natural one given the Gibbs states for the two separated systems. We denote it by $\langle\cdot\rangle_\Lambda$. We are interested in the expectation value $\langle s_X - \mathcal{S}_X^3 \rangle_\Lambda$ for some $X \subset \Lambda$. Since the trace is invariant under unitary transformations, we can apply on each site the unitary $(\mathcal{S}_x^1, \mathcal{S}_x^2, \mathcal{S}_x^3) \to (\mathcal{S}_x^1, s_x \mathcal{S}_s^2, s_x \mathcal{S}_x^3)$ and find

$$\sum_{s\in\Omega_\Lambda} \mathrm{Tr}\left(s_X - \mathcal{S}_X^3\right) \mathrm{e}^{-\mathscr{H}} = \sum_{s\in\Omega_\Lambda} \mathrm{Tr}\, s_X (1 - \mathcal{S}_X^3)\, \mathrm{e}^{\sum_{A\subset\Lambda} J_A^1 \mathcal{S}_A^1 + J_A^3 s_A (1+\mathcal{S}_A^3)} \tag{61}$$

The expression evaluated above is just the expectation value we are interested in multiplied by the partition function of the system—which is positive and therefore not useful in the evaluation of the sign of $\langle s_X - \mathcal{S}_X^3 \rangle_\Lambda$. By a Taylor expansion and by the property $\sum_{s\in\Omega_\Lambda} \prod_{x\in A} s_x^{n_x} \geq 0$ with $n_x \in \mathbb{N}$ for all $x \in \Lambda$ and any $A \subset \Lambda$, it is clear that the expression above is nonnegative. This implies that

$$\langle s_X \rangle_{\Lambda,\{J_A^3\}}^{\mathrm{Is}} - \langle \mathcal{S}_X^3 \rangle_{\Lambda,\mathcal{S}}^{\mathrm{qu}} = \langle s_X - \mathcal{S}_X^3 \rangle_\Lambda \geq 0. \tag{62}$$

This proves Eq. (59).

Acknowledgements The authors thank S. Bachmann and C.E. Pfister for useful comments.

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Dissipatively Generated Entanglement

Fabio Benatti

Abstract Given two non-interacting 2-level systems weakly coupled to an environment and thus evolving according to a statistically mixing dissipative reduced dynamics, we provide necessary and sufficient conditions for the generator of the time-evolution to entangle the two systems.

Keywords Entanglement • Markovian quantum evolutions • Open quantum systems

1 Introduction

Quantum systems always interact with the environment in which they are immersed; when the coupling to the environment is negligible, they evolve reversibly. Otherwise, when the interaction with the environment is weak, but cannot be neglected, quantum systems are called *open* [1, 2]. The weakness of the interaction allows one to derive a *reduced dynamics* that describes the noisy and dissipative effects due to the presence of the environment after it has been eliminated by tracing out its degrees of freedom. Usually, this operation yields an irreversible time-evolution characterised by memory effects that can be eliminated by suitable Markovian approximations that lead to master equations of the form

$$\partial_t \varrho_t = \mathbb{L}[\varrho_t] , \tag{1}$$

for all $t \geq 0$, where $\mathbb{L}$ is a time-independent generator. Assuming the system to be a d-level system, then $\varrho_t \in M_d(\mathbb{C})$ must be a (positive and normalized) $d \times d$ density matrix describing the state of the open quantum system at time $t \geq 0$.

Therefore, the dynamical maps $\Lambda_t = \mathrm{e}^{t\mathbb{L}}$ generated by (1) must preserve the positivity of any initial ϱ, so that the eigenvalues of $\varrho_t = \Lambda_t[\varrho] \geq 0$ might be interpretable as probabilities at all times $t \geq 0$; namely, Λ_t must be positivity

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A. Michelangeli, G. Dell'Antonio (eds.), *Advances in Quantum Mechanics*,
Springer INdAM Series 18, DOI 10.1007/978-3-319-58904-6_3

preserving, positive in short, for all $t \geq 0$. This condition is necessary but not sufficient to ensure the full physical consistency of Λ_t; indeed, one can always statistically couple an open quantum system S with another inert d-level system S, so that the states $\varrho \in M_d(\mathbb{C}) \otimes M_d(\mathbb{C})$ of the compound bipartite system $S + S$ would evolve under the action of a fully admissible dynamical map $\Lambda_t \otimes \mathrm{id}$. If the states ϱ were all of the form

$$\rho_{sep} = \sum_k \lambda_k \rho_k^{(1)} \otimes \rho_k^{(2)} , \quad \lambda_k \geq 0 , \sum_k \lambda_k = 1 , \tag{2}$$

with their correlations only due to the mixing with weights λ_k of the uncorrelated tensor products of constituent system states $\rho_k^{(1)} \otimes \rho_k^{(2)}$, the positivity of Λ_t would clearly be sufficient to guarantee that $\Lambda_t \otimes \mathrm{id}[\rho_{sep}] \geq 0$. However, not all bipartite states are expressible in a separable form as in (2): those which cannot are called *entangled* [3]. It turns out that, when Λ_t is positive, but not completely positive, there surely exists an entangled state $\varrho_{ent} \in M_d(\mathbb{C}) \otimes M_d(\mathbb{C})$ such that $\Lambda_t \otimes \mathrm{id}[\varrho_{ent}]$ assumes negative eigenvalues in the course of time [4]. Summarizing, complete positivity of Λ_t is necessary (and sufficient) to guarantee that both Λ_t and $\Lambda_t \otimes \mathrm{id}$ be positivity preserving and thus physically consistent.

In the Markovian case, the dynamical maps Λ_t are completely positive if and only if the generator is of the so-called Gorini-Kossakowski-Sudarshan-Lindblad form [5, 6]

$$\mathbb{L}[\varrho_t] = -i[H\, ,\, \varrho_t] + \sum_{j=1}^{d^2-1} K_{ij}\Big(F_i\, \varrho_t\, F_j^\dagger - \frac{1}{2}\Big\{F_j^\dagger F_i\, ,\, \varrho_t\Big\}\Big) , \tag{3}$$

with traceless matrices such that $\{F_j\}_{j=1}^{d^2-1}$, $\mathrm{Tr}(F_i^\dagger F_j) = \delta_{ij}$, which, together with $F_{d^2} = 1/\sqrt{d}$, constitute an orthonormal basis in $M_d(\mathbb{C})$ and the $(d^2-1) \times (d^2-1)$ matrix $K = [K_{ij}]$, known as *Kossakowski matrix*, being positive semi-definite.

Markovian semigroups of completely positive maps are used to describe decoherence processes detrimental to the persistence of non-classical correlations, like entanglement, and to their use to perform classically impossible informational tasks like teleportation and quantum cryptography [7]. However, not always the presence of an environment is negative; sometimes, it is also possible to engineer the environment in such a way that two non-directly interacting systems immersed in it become entangled [8–10].

For two 2-level systems, a sufficient condition for such a possibility to occur was provided in [9] in the case of a purely dissipative generator of the form

$$\mathbb{L}[\varrho_t] = -i[H\, ,\, \varrho_t] + \sum_{j,k=1}^{6} K_{j,k}\Big(S_j\, \varrho_t\, S_k - \frac{1}{2}\Big\{S_k S_j\, ,\, \varrho_t\Big\}\Big)$$

$$H = \sum_{j=1} H_j\, S_j\, , \qquad H_j = H_j^* \, ,$$

where $S_j = \sigma_j \otimes \mathbf{1}$ for $j = 1, 2, 3$, $S_j = \mathbf{1} \otimes \sigma_{j-3}$ for $j = 4, 5, 6$, with $\sigma_{1,2,3}$ the Pauli matrices and $\mathbf{1}$ the identity 2×2 matrix, and the hermitean Kossakowski matrix $K = [K_{jk}]$ is positive semi-dedefinite. Notice the absence in the above generator of operators pertaining simultaneously to the two qubits like $\sigma_i \otimes \sigma_j$. Then, the emergence of entanglement during the time-evolution may only be due to the mixing properties of the dissipation and not to dynamical effects.

In the following, we provide necessary and sufficient conditions for the above generator to create entanglement by focussing on just one part of the generator and proving the following result.

Theorem 1 *Let two* 2*-level systems immersed in a common environment evolve according to a master equation* $\partial_t \varrho_t = \mathbb{L}[\varrho_t]$ *generated by* $\mathbb{L}$ *as in (5). Given an initially separable state* ϱ_{sep}*, the generated dynamical maps* Λ_t *on* $M_2(\mathbb{C}) \otimes M_2(\mathbb{C})$ *turns it into an entangled state, if and only if so does the dynamics generated by*

$$\mathbb{Z}[\varrho] = -i\left(H - \frac{i}{2}\Gamma\right)\varrho \; + i\,\varrho\left(H + \frac{i}{2}\Gamma\right)$$

$$\Gamma = \sum_{j,k=1}^{6} K_{jk}\, S_k S_j \geq 0 \, .$$

2 Dissipative Entanglement Generation

The simplest introduction to the notion of entanglement is by means of two 2-level systems, or in the jargon of quantum information, by systems consisting of two qubits. We shall denote by $\{|i\rangle\}_{i=0}^{1}$ the orthonormal basis of the eigenvectors of σ_3 in the single qubit Hilbert space $\mathbb{C}^2$: $\sigma|i\rangle = (-)^i|i\rangle$.

Then, two qubit vector states $|\Psi_{12}\rangle \in \mathbb{C}^4$ are entangled if they cannot be written as tensor products $|\psi\rangle \otimes |\phi\rangle$ of single qubit vector states, the prototype of such states being the so-called symmetric state

$$|\Psi_+\rangle = \frac{|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle}{\sqrt{2}} \, . \tag{4}$$

Entanglement as a property of quantum states is strictly related to positive, but not completely positive maps on quantum observables [4, 11], the prototype of such maps being the transposition map $\mathbb{T}$ (defined with respect to the chosen representation). Indeed, the latter is a positive map as it does not alter the spectrum of the matrices on which it acts; however, the partial transposition $\mathbb{T}\otimes\mathrm{id}$, transposing only the first factor of a bipartite tensor product of operators, fails to be positive.

Indeed, the symmetric projector $P_+ = |\Psi_+\rangle\langle\Psi_+|$ changes from

$$P_+ = \frac{1}{2}\Big(|0\rangle\langle 0| \otimes |0\rangle\langle 0| + |1\rangle\langle 1| \otimes |1\rangle\langle 1| + |0\rangle\langle 1| \otimes |0\rangle\langle 1| + |1\rangle\langle 0| \otimes |1\rangle\langle 0|\Big)$$

into

$$\begin{aligned}&(\mathbb{T} \otimes \mathrm{id})[P_+] \\ &\quad = \frac{1}{2}\Big(|0\rangle\langle 0| \otimes |0\rangle\langle 0| + |1\rangle\langle 1| \otimes |1\rangle\langle 1| + |1\rangle\langle 0| \otimes |0\rangle\langle 1| + |0\rangle\langle 1| \otimes |1\rangle\langle 0|\Big)\end{aligned}$$

which has the anti-symmetric state

$$|\Psi_-\rangle = \frac{1}{\sqrt{2}}\Big(|0\rangle \otimes |1\rangle - |1\rangle \otimes |0\rangle\Big)$$

as eigenvector relative to the negative eigenvalue $-1/2$. Therefore, though $\mathbb{T}$ is a sensible, positivity preserving map on single qubits, its so-called lifting $\mathbb{T} \otimes \mathrm{id}$ fails to be such when acting on systems consisting of two qubits due to the existence of entangled states. In practice, transposition acts as a witness for the entanglement of P_+; actually for two qubits $\mathbb{T}$ is an exhaustive entanglement witness [12].

Theorem 2 *A state ϱ in $M_2(\mathbb{C}) \otimes M_2(\mathbb{C})$ is entangled if and only if it does not remain positive semi-definite under partial transposition, namely if and only if*

$$(\mathbb{T} \otimes \mathrm{id})[\varrho] \not\geq 0 \, .$$

The issue at stake in the following is the role of the dissipative part of the generator in Theorem 1,

$$\mathbb{L}[\varrho_t] = -i[H \, , \, \varrho_t] + \sum_{j,k=1}^{6} K_{jk}\Big(S_j\, \varrho_t\, S_k - \frac{1}{2}\Big\{S_k S_j \, , \, \varrho_t\Big\}\Big) \tag{5}$$

$$H = \sum_{j=1}^{6} H_j\, S_j \, , \qquad H_j = H_j^* \, , \tag{6}$$

with $S_j = \sigma_j \otimes \mathbf{1}$ for $j = 1, 2, 3$ and $S_j = \mathbf{1} \otimes \sigma_{j-3}$ for $j = 4, 5, 6$, in transforming an initial separable state (2) into an entangled state.

Notice that the Hamiltonian part splits into two terms acting independently on the two qubits and cannot thus entangle them, being thus only the dissipative contribution that can achieve it.

The generator can be subdivided into two terms: the first one, $\mathbb{Z}$, consists of a pseudo-commutator

$$\mathbb{Z}[\varrho] = -i\left(H - \frac{i}{2}\Gamma\right)\varrho \,+\, i\,\varrho\left(H + \frac{i}{2}\Gamma\right) \tag{7}$$

$$\Gamma = \sum_{j,k=1}^{6} K_{jk}\, S_k\, S_j \,, \tag{8}$$

with respect to a non-hermitean Hamiltonian. Since $\Gamma \geq 0$ because the Kossakowski matirx $K \geq 0$, $\mathbb{Z}$ generates a damped quantum dynamics sending projections into non-normalized projections:

$$\mathrm{e}^{t\mathbb{Z}}[|\psi\rangle\langle\psi|] = \mathrm{e}^{-it(H-i\Gamma/2)}\,|\psi\rangle\langle\psi|\,\mathrm{e}^{it(H+i\Gamma/2)} \,. \tag{9}$$

As to the remaining contribution to the generator,

$$\mathbb{B}[\varrho] = \sum_{j,k=1}^{6} K_{jk}\, S_j\, \varrho\, S_k \,, \tag{10}$$

by using the spectral representation of the Kossakowski matrix $K = [K_{jk}] \geq 0$, it can be expressed in the standard Kraus-Stinespring form of completely positive maps

$$\mathbb{B}[\varrho] = \sum_{\ell=1}^{6} V_\ell\, \varrho\, V_\ell^\dagger \,. \tag{11}$$

Unlike the damping term, $\mathbb{B}$ transforms projectors into mixtures of projections, thus representing a so-called *noisy channel*[1] The standard lore has it that entanglement comes from mutual interactions between the qubits described by the Hamiltonian H, while the remaining dissipative contributions are responsible for its depletion in time due to damping and noise.

This conclusion is not always true: suitably engineered dissipative dynamics may lead to dissipatively generated entanglement even in absence of direct qubit interactions and this entanglement can also persist asymptotically in time [8–10, 13].

Regarding the generator (5), in [9] a sufficient condition for entanglement generation was provided that was related to the structure of the 6×6 Kossakowski matrix $C = [C_{jk}]$. In the following, we shall show that the actual source of entanglement might only be due to the pseudo-commutative contribution, the noise term being unable to counteract this fact.

[1] Notice that the trace is preserved since $\mathrm{Tr}(\mathbb{B}[\varrho] + \mathrm{Tr}(\mathbb{Z}[\varrho]) = 0$.

2.1 Checking Entanglement Generation

In order to ascertain whether $\Lambda_t = e^{t\mathbb{L}}$ acting on an initially separable two qubit state may or not entangle it in the course of time, we base our strategy upon Theorem 2 and the following observations:

- since general separable density matrices are liner convex combination of pure separable states, one need just study the action of Λ_t on projections of the form $P_\psi \otimes P_\phi$;
- one need check whether there exist separable projections such that

$$(\mathbb{T} \otimes \mathrm{id}) \circ \Lambda_t[P_\psi \otimes P_\phi] \not\geq 0 \; ;$$

- one can focus upon very small times; indeed, in order to become negative an eigenvalue of $(\mathbb{T} \otimes \mathrm{id}) \circ \Lambda_t[P_\psi \otimes P_\phi]$ must first become zero at some time $t_* \geq 0$ and then < 0 at $t_* + \varepsilon$, for $\varepsilon > 0$ sufficiently small.

Then, the maps Λ_t are entanglement generating if and only if there exists a separable pure state projection $P_\psi \otimes P_\phi$ onto $|\psi\rangle \otimes |\phi\rangle$ such that, at first order in t,

$$(\mathbb{T} \otimes \mathrm{id}) \circ \Lambda_t[P_\psi \otimes P_\phi] \simeq P_{\psi^*} \otimes P_\phi + t\,(\mathbb{T} \otimes \mathrm{id}) \circ \mathbb{L}[P_\psi \otimes P_\phi] \tag{12}$$

is not positive semi-definite. Here, $|\psi^*\rangle$ is the conjugate of $|\psi\rangle$ with respect to the orthonormal basis where σ_3 is diagonal so that, under transposition, $\sigma_j^T = \epsilon_j\,\sigma_j$ with ϵ_j, $j = 1, 2, 3$, determined by

$$\sigma_1^T = \sigma_1 \; , \qquad \sigma_2^T = -\sigma_2 \; , \qquad \sigma_3^T = \sigma_3 \; . \tag{13}$$

For later use, we then introduce the following 3×3 diagonal matrix

$$\mathscr{E} := \begin{pmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_2 & 0 \\ 0 & 0 & \epsilon_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \; . \tag{14}$$

The lack of positive semi-definiteness of $(\mathbb{T} \otimes \mathrm{id}) \circ \Lambda_t[P_\psi \otimes P_\phi]$ can be studied by considering its expectation values with respect to an (entangled) pure state $|\Psi\rangle$ orthogonal to $|\psi^*\rangle \otimes |\phi\rangle$, so that

$$\langle\Psi|(\mathbb{T} \otimes \mathrm{id}) \circ \Lambda_t[P_\psi \otimes P_\phi]\Psi\rangle \simeq t\,\langle\Psi|(\mathbb{T} \otimes \mathrm{id}) \circ \mathbb{L}[P_\psi \otimes P_\phi]|\Psi\rangle =: \Delta(t) \; . \tag{15}$$

Remark 1 The vector $|\Psi\rangle$ must be entangled: if $P_\Psi = |\Psi\rangle\langle\Psi| = P_{\psi_1} \otimes P_{\psi_2}$, where $P_{\psi_1} = |\psi_1\rangle\langle\psi_1|$, $P_{\psi_2} = |\psi_2\rangle\langle\psi_2|$, by transferring the partial transposition from

$\Lambda_t[P_\psi \otimes P_\phi]$ onto P_Ψ, one would obtain

$$\langle\Psi|(\mathbb{T}\otimes \mathrm{id})\circ\Lambda_t[P_\psi\otimes P_\phi]\Psi\rangle = \mathrm{Tr}\Big((\mathbb{T}\otimes\mathrm{id})[P_\Psi]\Lambda_t[P_\psi\otimes P_\phi]\Big) = \langle\psi_1^*\otimes\psi_2|\Lambda_t[P_\psi\otimes P_\phi]\psi_1^*\otimes\psi_2\rangle \geq 0\,,$$

where $|\psi_1^*\rangle$ is the conjugate of $|\psi_1\rangle$ that comes from transposing P_{ψ_1} in the fixed representation.

The action of the partial transposition on the generator $\mathbb{L}$ is better understood by rewriting the 6×6 Kossakowski matrix $K = [K_{jk}] \geq 0$ as

$$K = \begin{pmatrix} A & B \\ B^\dagger & C\end{pmatrix} \tag{16}$$

with $A, B, C \in M_3(\mathbb{C})$ and A and C necessarily positive semi-definite, and then, recasting Γ as

$$\Gamma = \sum_{j,k=1}^{3} A_{jk}\,\sigma_k\sigma_j\otimes\mathbf{1} + \sum_{j,k=1}^{3} C_{jk}\,\mathbf{1}\otimes\sigma_k\sigma_j + \sum_{j,k=1}^{3} B_{jk}\,\sigma_j\otimes\sigma_k + \sum_{j,k=1}^{3} B^*_{kj}\,\sigma_k\otimes\sigma_j\,, \tag{17}$$

and $\mathbb{B}[\varrho]$ in (10) as

$$\mathbb{B}[\varrho] = \sum_{j,k=1}^{3} A_{jk}\,\sigma_j\otimes\mathbf{1}\,\varrho\,\sigma_k\otimes\mathbf{1} + \sum_{j,k=1}^{3} C_{jk}\,\mathbf{1}\otimes\sigma_j\,\varrho\,\mathbf{1}\otimes\sigma_k \tag{18}$$

$$+ \sum_{j,k=1}^{3} B_{jk}\,\sigma_j\otimes\mathbf{1}\,\varrho\,\mathbf{1}\otimes\sigma_k + \sum_{j,k=1}^{3} B^*_{jk}\,\mathbf{1}\otimes\sigma_k\,\varrho\,\sigma_j\otimes\mathbf{1}\,. \tag{19}$$

Then, using (13) one computes

$$(\mathbb{T}\otimes\mathrm{id})\circ\mathbb{Z}[P_\psi\otimes P_\phi] = -i\sum_{j=1}^{3} H_j\epsilon_j\,\big[P_{\psi^*}\,,\,\sigma_j\big]\otimes P_\phi - i\sum_{j=4}^{6} H_j\,P_{\psi^*}\otimes\big[\sigma_j\,,\,P_\phi\big] \tag{20}$$

$$-\frac{1}{2}\sum_{j,k=1}^{3} A_{jk}\epsilon_j\epsilon_k\,\big\{P_{\psi^*}\,,\,\sigma_j\sigma_k\big\}\otimes P_\phi - \frac{1}{2}\sum_{j,k=1}^{3} C_{jk}\,P_{\psi^*}\otimes\big\{\sigma_k\sigma_j\,,\,P_\phi\big\} \tag{21}$$

$$-\sum_{j,k=1}^{3}\mathscr{R}e(B_{jk})\,\epsilon_j\Big(\sigma_j\otimes\mathbf{1}\,P_{\psi^*}\otimes P_\phi\,\mathbf{1}\otimes\sigma_k + \mathbf{1}\otimes\sigma_k P_{\psi^*}\otimes P_\phi\,\sigma_j\otimes\mathbf{1}\Big)\,, \tag{22}$$

and

$$(\mathbb{T}\otimes \mathrm{id})\circ \mathbb{B}[P_\psi \otimes P_\phi] = \sum_{j,k=1}^{3} A_{jk}\epsilon_j\epsilon_k\, \sigma_k \otimes \mathbf{1}\left(P_{\psi^*}\otimes P_\phi\right)\sigma_j \otimes \mathbf{1} \tag{23}$$

$$+\sum_{j,k=1}^{3} C_{jk}\,\mathbf{1}\otimes \sigma_j\left(P_{\psi^*}\otimes P_\phi\right)\sigma_k\otimes \mathbf{1} \tag{24}$$

$$+\sum_{j,k=1}^{3} B_{jk}\epsilon_j\left(P_{\psi^*}\otimes P_\phi\right)\sigma_j\otimes\sigma_k \tag{25}$$

$$+\sum_{j,k=1}^{3} B^*_{jk}\,\epsilon_j\,\sigma_j\otimes\sigma_k\left(P_{\psi*}\otimes P_\phi\right). \tag{26}$$

Notice that, by putting together the above expressions, it thus turns out that partial transposition transforms the generator $\mathbb{L}$ into a linear map $\mathbb{N} := (\mathbb{T}\otimes\mathrm{id})\circ\mathbb{L}\circ(\mathbb{T}\otimes\mathrm{id})$ such that

$$\mathbb{N}[\varrho] = -i[\widetilde{H}, \varrho] + \sum_{j,k=1}^{6} N_{jk}\left(S_j\,\varrho\,S_k - \frac{1}{2}\left\{S_k\,S_j\,,\,\varrho\right\}\right) \tag{27}$$

$$\widetilde{H} := -\sum_{j=1}^{3}\epsilon_j H_j\,S_j + \sum_{j=4}^{6} H_j\,S_j + \sum_{j,k=1}^{3}\epsilon_j\,\mathscr{I}m(B_{jk})\,\sigma_j\otimes\sigma_k \tag{28}$$

$$N = [N_{jk}] := \mathscr{E}\begin{pmatrix} A^T & (B+B^*)/2 \\ (B^\dagger + B^T)/2 & C\end{pmatrix}\mathscr{E}\,, \tag{29}$$

where $\mathscr{E}$ is the matrix introduced in (14), B^* is the matrix with entries B^*_{jk} and $B+B^*$ is the 3×3 matrix with real entries $2\,\mathscr{R}e(B_{jk})$.

Remark 2 The linear map $\mathbb{N}$ generates a semigroup of maps $\mathscr{N}_t = \exp(t\mathbb{N})$. Since, the matrix $N = [N_{jk}]$ need not be positive semi-definite, the partially transposed semigroup need not have any physical meaning.

We now expand $|\Psi\rangle$ along the orthonormal basis of $\mathbb{C}^2\otimes\mathbb{C}^2$ given by the orthogonal pairs $\{|\psi^*\rangle, |(\psi^*)^\perp\rangle\}$ and $\{|\phi\rangle, |\phi^\perp\rangle\}$,

$$|\Psi\rangle = a\,|\psi^*\rangle\otimes|\phi\rangle + b\,|(\psi^*)^\perp\rangle\otimes|\phi\rangle + c\,|(\psi^*)^\perp\rangle\otimes|\phi^\perp\rangle\,. \tag{30}$$

Then, the orthogonality between $|\Psi\rangle$ and $|\psi^*\rangle \otimes |\phi_1\rangle$ reduces to one the contributions to $\Delta(t)$ in (15):

$$\Delta(t) = t\langle\Psi|\mathbb{N}[P_{\psi^*} \otimes P_\phi]|\Psi\rangle = \sum_{j,k=1}^{6} \langle\Psi|\, S_j\, P_{\psi^*} \otimes P_\phi\, S_k\, |\Psi\rangle\ . \tag{31}$$

From these considerations the following result ensues [14]).

Proposition 1 *The dissipative semigroup of completely positive maps* $\Lambda_t = \exp(t\mathbb{L})$*, with* $\mathbb{L}$ *as in (5), is entanglement generating if and only if there exist vectors* $|\psi\rangle\,,\ |\phi\rangle \in \mathbb{C}^2$ *such that* $\Delta(t)$ *in (31) becomes negative at some* $t > 0$.

2.2 Case 1: $\mathbb{Z}$ Does Not Generate Entanglement

We shall first show that, if $\mathbb{Z}$ in (7) and (8) cannot generate entanglement, then $\mathbb{B}$ in (10) is such that $\mathbb{L} = \mathbb{Z} + \mathbb{B}$ cannot either.

Proposition 2 *Suppose the pseudo-commutator* $\mathbb{Z}$ *in (7) does not entangle any initial separable projection* $P_\psi \otimes P_\phi$*; then, in (29),* $B + B^* = 0$.

Proof The argument leading to Proposition 1 applies also when the time-evolution is generated by $\mathbb{Z}$ only, the difference being that the evolving state is a non-normalized projection (see (9)). Then, to the corresponding quantity $\Delta(t)$ there contributes only the term (22), so that $\Delta(t)$ in (15) becomes

$$\begin{aligned}
\Delta(t) &= t\,\langle\Psi|(\mathbb{T}\otimes \mathrm{id})\circ \mathbb{Z}[P_{\psi^*}\otimes P_\phi]|\Psi\rangle \\
&= -2\,\mathscr{I}m\Big(a\,b^* \sum_{j,k=1}^{3} \varepsilon_j\,\mathscr{R}e(B_{jk})\,\langle\psi^*|\sigma_j(\psi^*)^\perp\rangle\langle\phi^\perp|\sigma_k\phi\rangle\Big) \\
&= -2\mathscr{I}m\left(a\,b^*\left\langle u\,\middle|\,\mathscr{E}\,\frac{B+B^*}{2}\,v\right\rangle\right)
\end{aligned}$$

where $|\Psi\rangle$ is the entangled state in (30) orthogonal to $|\psi^*\rangle \otimes |\phi\rangle$ and

$$|u\rangle = \begin{pmatrix} \langle(\psi^*)^\perp|\sigma_1\psi^*\rangle \\ -\langle(\psi^*)^\perp|\sigma_2\psi^*\rangle \\ \langle(\psi^*)^\perp|\sigma_3\psi^*\rangle \end{pmatrix}\ , \quad |v\rangle = \begin{pmatrix} \langle\phi^\perp|\sigma_1\phi\rangle \\ \langle\phi^\perp|\sigma_2\phi\rangle \\ \langle\phi^\perp|\sigma_3\phi\rangle \end{pmatrix}\ .$$

The assumption that $\mathbb{Z}$ generate no entanglement amounts to the request that $\Delta(t)$ be non negative for all possible $a, b \in \mathbb{C}$ and all $|u\rangle, |v\rangle$. This in turn asks for

$$\left\langle u \left| \mathscr{E} \frac{B+B^*}{2} v \right\rangle = 0\right.$$

for all $|u\rangle\,|v\rangle \in \mathbb{C}^3$. By choosing $|\psi\rangle$ to be an eigenstate of σ_1, then of σ_2 and finally of σ_3, one gets three linearly independent $|u\rangle \in \mathbb{C}^3$ and analogously for $|v\rangle$. Then, the request that $\Delta(t)$ be non-negative for all $|\psi\rangle$, $|\phi\rangle \in \mathbb{C}^2$, together with the invertibility of the matrix $\mathscr{E}$ in (14) yields the result.

Corollary 1 *If $\mathbb{Z}$ does not generate entanglement, neither does $\mathbb{L}$ in (5).*

Proof Given the hypothesis, the previous proposition makes diagonal the matrix $N = [N_{ij}]$ in (29),

$$N = \begin{pmatrix} \mathscr{E} A^T \mathscr{E} & 0 \\ 0 & C \end{pmatrix} .$$

Since $\mathbb{L}$ generates a semigroup of completely positive maps, then, by Gorini-Kossakowski-Sudarshan-Lindblad theorem (see (3)), the Kossakowski matrix K must be positive semi-definite, whence $\mathscr{E} A^T \mathscr{E}$ and C are both positive semi-definite matrices. Then, by the same theorem, the partially transposed generator $\mathbb{N}$ in (27) also generates a semigroup of completely positive maps $\mathscr{N}_t = \exp(t\mathbb{N})$ (see Remark 2), so that $\mathscr{N}_t[P_{\psi^*} \otimes P_\phi]$ is always positive semi-definite for all $t \geq 0$ and $\Delta(t)$ in (31) cannot become negative.

2.3 *Case 2: $\mathbb{Z}$ Generates Entanglement*

Without restricting to the specific generator $\mathbb{L}$ in the previous section, we now cast the master Eq. (1) as an equation for the dynamical maps Λ_t, $\partial_t \Lambda_t = \mathbb{L} \circ \Lambda_t$, and introduce the Laplace transform of the solution Λ_t,

$$\widetilde{\Lambda}_s := \int_0^{+\infty} \mathrm{d}t \, \mathrm{e}^{-st} \, \Lambda_t \qquad s \geq 0 \, . \tag{32}$$

Then, the master equation translates into

$$\begin{aligned} \widetilde{\Lambda}_s &= \frac{1}{s-\mathbb{L}} = \frac{1}{s-\mathbb{Z}-\mathbb{B}} = \frac{1}{s-\mathbb{Z}} + \frac{1}{s-\mathbb{Z}} \Big(s-\mathbb{Z}-(s-\mathbb{Z}-\mathbb{B}) \Big) \frac{1}{s-\mathbb{Z}-\mathbb{B}} \\ &= \frac{1}{s-\mathbb{Z}} \sum_{k=0}^{+\infty} \left(\mathbb{B} \frac{1}{s-\mathbb{Z}} \right)^k . \end{aligned} \tag{33}$$

One thus sees that if Λ_t, $t \geq 0$, is positive, respectively completely positive, such is also the Laplace transform $\widetilde{\Lambda}_s$, $s \geq 0$, since the latter is an integral of positive, respectively completely positive maps weighted by positive factors. Moreover, the same is true of

$$(-)^k \frac{\mathrm{d}^k}{\mathrm{d}s^k} \widetilde{\Lambda}_s = \int_0^{+\infty} \mathrm{d}t \, t^k \, \Lambda_t \qquad \forall \, k \geq 0 \, . \tag{34}$$

A theorem of Bernstein [15] asserts that the latter ones are not only necessary, but also sufficient conditions for Λ_t to be positive, respectively completely positive.

Remark 3 The Laplace transform of the dynamics has been thoroughly used in dealing with the complete positivity of dynamical maps outside the Markovian regime when they are generated by time-dependent master equations of the form

$$\partial_t \varrho_t = \int_0^t \mathrm{d}\tau \, \mathbb{K}_{t-\tau}[\varrho_\tau] \, , \qquad \Lambda_{t=0} = \mathrm{id} \, , \tag{35}$$

where $\mathbb{K}_t$ is a suitable kernel. In this case, not so many results are available regarding the form it ought to have in order to generate a complete positive dynamics. Postulating a kernel of the form $\mathbb{K}_t := \mathbb{Z}_t + \mathbb{B}_t$ satisfying trace preservation (see footnote 1), the use of (33) allowed the construction of *legitimate pairs* $(\mathbb{Z}_t \, , \, \mathbb{B}_t)$, such that the generated dynamics is completely positive [15]. In this approach, it clearly emerges the pivotal role played by the the $\mathbb{Z}_t$ term with respect to $\mathbb{B}_t$ in ensuring the complete positivity of the generated time-evolution.

Since we are dealing with two qubits, the linear maps $\mathbb{Z}$ and $\mathbb{B}$ have finite norms $\|\mathbb{Z}\|$ and $\|\mathbb{B}\|$ on $M_4(\mathbb{C})$. Then, from (33) one can estimate, for $s > \|\mathbb{Z}\| + \|\mathbb{B}\|$,

$$\left\| \widetilde{\Lambda}_s - \frac{1}{s - \mathbb{Z}} \right\| \leq \sum_{k=1}^{\infty} \|\mathbb{B}\|^k \left\| \frac{1}{s - \mathbb{Z}} \right\|^{k+1} \leq \frac{\|\mathbb{B}\|}{(s - \|\mathbb{B}\|)^2} \, \frac{1}{1 - \frac{\|\mathbb{B}\|}{s - \|\mathbb{Z}\|}} \, ,$$

whence, for large $s \geq 0$,

$$\widetilde{\Lambda}_s = \frac{1}{s - \mathbb{Z}} + o\left(s^{-1}\right) \, , \qquad (-)^k \frac{\mathrm{d}^k}{\mathrm{d}s^k} \widetilde{\Lambda}_s = \frac{k!}{(s - \mathbb{Z})^{k+1}} + o\left(s^{-(k+1)}\right) \, . \tag{36}$$

Applying these considerations, we can prove the following result.

Proposition 3 *Consider a semigroup of completely positive maps $\Lambda_t = \exp(t\mathbb{L})$, $t \geq 0$, on the state space of two qubits, with $\mathbb{L} = \mathbb{Z} + \mathbb{B}$ as in (3). Then, if $\mathbb{Z}$ generates entanglement, so does $\mathbb{L}$.*

Proof Since $\mathbb{Z}$ generates entanglement, the dynamical maps $\gamma_t := \exp(t\mathbb{N}_Z)$, with $\mathbb{N}_Z := (\mathbb{T} \otimes \mathrm{id}) \circ \mathbb{Z} \circ (\mathbb{T} \otimes \mathrm{id})$, cannot be positive. Indeed, there must exist an initial separable projection $P_\psi \otimes P_\phi$ such that $\gamma_t[P_\psi \otimes P_\phi]$ becomes entangled at some

$t > 0$. Thus, Theorem 2 together with the fact that

$$(\mathbb{T} \otimes \mathrm{id}) \circ \mathrm{e}^{t\mathbb{Z}} \circ (\mathbb{T} \otimes \mathrm{id}) = \mathrm{e}^{t\mathbb{N}_Z} ,$$

and $((\mathbb{T} \otimes \mathrm{id}))^2 = \mathrm{id}$ implies that

$$(\mathbb{T} \otimes \mathrm{id}) \circ \mathrm{e}^{t\mathbb{Z}}[P_\psi \otimes P_\phi] = \gamma_t[P_{\psi^*} \otimes P_\phi]$$

is no longer positive semi-definite. Then, going to the Laplace trasform $\widetilde{\gamma}_t$, Bernstein theorem (see (34)) implies that there must exist an integer $k \geq 0$ such that

$$(-)^k \frac{\mathrm{d}^k}{\mathrm{d}s^k} \widetilde{\gamma}_s = \frac{k!}{(s - \mathbb{N}_Z)^{k+1}}$$

is not a positive map. Let us now consider the full generator $\mathbb{L} = \mathbb{Z} + \mathbb{B}$ and its partially transposed partner

$$\mathbb{N} = (\mathbb{T} \otimes \mathrm{id}) \circ \mathbb{L} \circ (\mathbb{T} \otimes \mathrm{id}) = \mathbb{N}_Z + \mathbb{N}_B , \qquad \mathbb{N}_B := (\mathbb{T} \otimes \mathrm{id}) \circ \mathbb{B} \circ (\mathbb{T} \otimes \mathrm{id}) .$$

Then, regarding the Laplace transform $\widetilde{\mathscr{N}}_s$ of the maps $\mathscr{N}_t = \mathrm{e}^{t\mathbb{N}}$, from the asymptotic behaviour (36) for large $s \geq 0$, one can conclude that also

$$(-)^k \frac{\mathrm{d}^k}{\mathrm{d}s^k} \widetilde{\mathscr{N}}_s = \frac{k!}{(s - \mathbb{N}_Z)^{k+1}} + o\left(s^{-(k+1)}\right)$$

cannot be a positive map for sufficiently large $s \geq 0$. Therefore, again by Bernstein theorem, $\mathscr{N}_t = (\mathbb{T} \otimes \mathrm{id}) \circ \Lambda_t$ cannot be positive and thus Λ_t must be entanglement generating for some $t \geq 0$.

3 Conclusions

Two qubits have been considered in weak interaction with a common environment that makes them evolve according to a dissipative semigroup of completely positive maps $\Lambda_t = \exp(t\mathbb{L})$ that do not provide mediated interaction between the two open quantum systems, but only statistically mix them. The paper provides necessary and sufficient conditions on the generator $\mathbb{L} = \mathbb{Z} + \mathbb{B}$ for the dynamical maps Λ_t to be able to entangle initial separable states. As is the case with master equations generating semigroups of completely positive maps, the generator $\mathbb{L}$ consists of two terms: a pseudo-commutative term $\mathbb{Z}$ responsible for a damped time-evolution transforming vector states into non-normalized vector states and a noise term $\mathbb{B}$ transforming vector states into mixtures of projections. A Laplace transform technique has been used that reduced the problem to the discussion of the properties of the pseudo-commutator $\mathbb{Z}$ showing that if the latter alone generates entanglement so does $\mathbb{L}$ and vice versa. As shortly mentioned in Remark 3, the Laplace transform had been used in [15] to study the complete positivity of the maps generated by a master equation with a time-dependent memory kernel $\mathbb{K}_t = \mathbb{Z}_t + \mathbb{B}_t$. There, it became apparent the prominence of the role of the pseudo-commutator $\mathbb{Z}_t$ in fixing the properties of the generator $\mathbb{K}_t$. The result in Theorem 1 confirms such an evidence in a memory-less context and in relation to entanglement generation.

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Abelian Gauge Potentials on Cubic Lattices

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Abstract The study of the properties of quantum particles in a periodic potential subjected to a magnetic field is an active area of research both in physics and mathematics, and it has been and is yet deeply investigated. In this chapter we discuss how to implement and describe tunable Abelian magnetic fields in a system of ultracold atoms in optical lattices. After reviewing two of the main experimental schemes for the physical realization of synthetic gauge potentials in ultracold set-ups, we study cubic lattice tight-binding models with commensurate flux. We finally discuss applications of gauge potentials in one-dimensional rings.

Keywords Abelian gauge potentials • Lattice models • Quantum entanglement • Quantum transfer • Ultracold atoms

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A. Michelangeli, G. Dell'Antonio (eds.), *Advances in Quantum Mechanics*,
Springer INdAM Series 18, DOI 10.1007/978-3-319-58904-6_4

1 Introduction

The study of the dynamics of a quantum particle in a magnetic field is a fascinating subject of perduring interest both in physics and mathematics literature. The quantization of energy levels giving rise to the Landau levels is at the basis of our understanding of integer and fractional quantum Hall effects [11, 13, 39, 66, 77] and its higher-dimensional counterparts and generalizations, including topological insulators [14, 19, 67]. The use of vector potentials in quantum mechanics is associated in itself to very interesting consequences, such as the purely quantum mechanical interference in the Aharonov-Bohm effect [3]. On the other side, the mathematical formalism for a particle in a magnetic field has been developed and refined along the time, based on the rigorous definition of Schrödinger operators with magnetic fields [10]. An important role is played by the construction of families of observables in the presence of gauge fields relying on the progresses in gauge covariant pseudodifferential calculus [42] and the C^*-algebraic formalism [58] (see for a review Ref. [57]). A major area of research in the field of single-particle and many-body properties in the presence of a magnetic field is provided by the study of the effects of periodic potentials. The interplay of the magnetic field and the discreteness induced by the lattice provides a paradigmatic system for the study of incommensurability effects [12, 38] and it results in an energy spectrum exhibiting a fractal structure, referred to as the Hofstadter butterfly [38]. Very interesting examples of the analysis of the so-called colored gaps can be found in [9, 68], while a discussion of the colored Hofstadter butterflies in honeycomb lattices can be found in [2].

The study of the Hofstadter Hamiltonian attracted in the years a sparkling activity, also due to its connections with the one-dimensional Harper model [36]. A concise, but very clear discussion is presented in [71], where it is shown how the Schrödinger equation for an electron in a magnetic field in the presence of a two-dimensional periodic potential can be mapped in a one-dimensional quasiperiodic equation. A derivation of Harper and Hofstadter models in the context of effective models for the conductance in magnetic fields was presented in [22], while a treatment of the Schrödinger operator in two dimensions with a periodic potential and a strong constant magnetic field perturbed by slowly varying non-periodic scalar and vector potentials has been recently discussed in [28]. A remarkable motivation for the studies of a two-dimensional electron gas in a uniform magnetic field and a periodic substrate potential is as well coming from the connection with topological invariants, as one can see from the study of the Hall conductance [72].

The theoretical studies on properties of lattice systems in a periodic potential found a experimental matching in the active research of solid-state realizations of the Hofstadter and related Hamiltonians. This effect has never been observed so far in a natural crystal due to the fact that a very large magnetic field would be required, however signatures of the Hofstadter bands has been observed in artificial superlattices [21, 27, 29, 59, 65]. This activity found recently a counterpart in the field of cold atoms, where it has been possible to load a neutral atomic gas in an optical lattice and simulate by external lasers an artificial magnetic potential [5, 60]. Given the fact that ultracold atoms, due to the high level of control and tunability of parameters [64], are an ideal physical setup in which perform quantum simulation [15], these and related experimental achievements opened the way to study a variety of lattice systems in a magnetic potential. In particular one can load on the lattice interacting bosonic and/or fermionic atoms, control the parameters of the lattice, use several components in each lattice site [54] and implement a variety of lattices of different dimensionalities (not only $D = 2$, but also $D = 1$ and $D = 3$).

The rationale of this Chapter is to report an introduction to the different ways to implement artificial magnetic potentials in the presence of a controllable lattice, with the goal to create a link with the many available results in theoretical and mathematical physics. From the other side we think that the variety of lattice models in magnetic fields implementable with ultracold gases may be a context in which test and apply techniques from the mathematical literature, and motivate further analytical and rigorous results, starting from the treatment of three-dimensional fermionic lattice systems. With these objectives, we then present in Sect. 2 a discussion on several different ways of realizing artificial magnetic fluxes in optical lattice systems. In Sects. 3 and 4 we present two possible applications of the results presented in Sect. 2 both to illustrate the versatility of possible uses of artificial magnetic potentials and to show results for $3D$ and $1D$ lattices. In Sect. 3 we review and study cubic lattice tight-binding models with a commensurate Abelian flux, also presenting results for the case of anisotropic fluxes. In Sect. 4 we consider $1D$ rings pierced by a magnetic field discussing how the latter can enhance the quantum state transfer and the entanglement entropy in the system.

We acknowledge several discussions we had along the years on the subjects treated in this chapter with several people, and special acknowledgements go to M. Aidelsburger, E. Alba, T. Apollaro, H. Buljan, A. Celi, I. C. Fulga, N. Goldman, G. Gori, M. Mannarelli, G. Mussardo, G. Panati, H. Price, M. Rizzi, P. Sodano and A. Smerzi. S. P. is supported by a Rita Levi-Montalcini fellowship of MIUR.

2 Realization of Artificial Magnetic Fluxes in Optical Lattice Systems

In the last 10 years many experiments with ultracold atoms demonstrated the possibility of realizing artificial magnetic fluxes trapped in two-dimensional optical lattices. Similar setups pave the way for a systematic study of topological phases of matter in the highly controllable environment provided by ultracold atoms [15]. Such experiments offer, on one side, the possibility of reaching regimes that are hardly achievable in solid state devices and, on the other, to verify the emergence of topological phenomena through observables typical of ultracold gases, such as the motion of the center of mass of the system, or the momentum distribution of the atoms [64]. The measurement of these quantities therefore provides useful tools to detect the appearance of topological phases of matter which are complementary to the usual transport measurements performed in solid state platforms.

The main result which enabled the experimental study of topological models in ultracold atomic systems was the realization of artificial gauge potentials. In this framework, we speak about *artificial* (or *synthetic*) gauge potentials because ultracold atoms are neutral, therefore their motion is not directly affected by the presence of a true electromagnetic field. Despite that, however, it turned out to be possible to engineer systems in which the dynamics of the slow and low-energy degrees of freedom can be described by an effective Hamiltonian in which the free, non-interacting, part is the one of a free-particle in a magnetic field. An interesting point to be observed is that the obtained Hamiltonian, featuring the presence of an artificial magnetic field, is interacting, with the interaction term tunable by e.g. Feshbach resonances or by acting on the geometry of the system. At the same time, typically, as we are going to discuss in the following, the synthetic field does not depend on the interactions or on the density of the system, being in a word a single-particle effect.

An efficient way to implement a synthetic gauge potential $\mathbf{A}$ giving rise to an artificial, static magnetic field $\mathbf{B} \propto \nabla \times \mathbf{A}$, is to implement with ultracold atoms in optical lattice a tight-binding Hamiltonian with hopping amplitudes which are, in general, complex and whose phases depend on the position. To be more clear, we point out that the implementation of synthetic gauge potentials in lattices relies on the well-established experimental successes in the quantum simulation of tight-binding Hamiltonians for both bosons and fermions [15].

For ultracold bosons, if a condensate is loaded in an optical lattice, then one can expand the condensate wavefunctions in the basis of the Wannier functions and obtain a discrete nonlinear Schrödinger (DNLS) equation [73]. The coefficient of the nonlinear term in the DNLS equation is proportional to the s-wave scattering length a and in general the coefficients of the DNLS equation depend on integrals of the Wannier functions. For $a = 0$ (i.e., for an effectively non-interacting condensate) one gets the discrete linear Schrödinger, which is nothing but the tight-biding model for which one can apply consolidated numerical analyses [55] and rigorous [16] techniques for the definition and determination of the Wannier functions and their behaviour. When $a \neq 0$ a rigorous theory of (nonlinear) Wannier functions does not exist, and the semiclassical equations of motion should be modified as a consequence of the existence of the nonlinearity. The development of a rigorous extension of Wannier functions in the presence of nonlinearity is a challenging mathematical problem for the future. We think this independently from the fact that an approximate determination of the Wannier functions (see e.g. for a variational approach in [18, 74, 75]) typically works very well to describe the experimental results when the laser intensity, i.e. the strength of the periodic potential, is large enough, also when the system approaches the superfluid-Mott transition and/or the gas is not longer condensate due to the presence of strong interactions [40]. Similar considerations apply for ultracold fermions: when there is in average no more than one particle per well and only the lowest band is occupied, a single-band tight-binding approximation works very well both when the dilute fermionic gas is polarized (corresponding to $a = 0$) and when more species or levels of fermions are present. In the following we consider tight-binding models describing ultracold atoms in optical lattices, sticking to the non-interacting limit and discussing how to simulate artificial gauge potentials in such systems. We alert anyway the reader that, albeit non-rigorous, the experimental techniques to implement synthetic magnetic field are the same also for interacting particles, even though the interacting terms may modify or generate additional coefficients in the tight-binding model and introduce corrections to the results obtained with the Peierls substitution [63].

To fix the notation, let us consider a lattice whose sites are denoted by $\mathbf{r}$: for a cubic D-dimensional lattice we have $\mathbf{r} \in \mathbb{Z}^D$. By using the Peierls substitution to take into account the effect of the magnetic field [45, 53, 63], the Hamiltonian we consider then reads

$$H(\{\phi\}) = -\sum_{\mathbf{r},\hat{j}} w_{\hat{j}}\, c^{\dagger}_{\mathbf{r}+\hat{j}}\, e^{i\phi_j(\mathbf{r})} c_{\mathbf{r}} + \text{H.c.}\,, \tag{1}$$

where $\hat{j}$ are unitary vectors characterizing the links of the lattice, $w_{\hat{j}}$ are the hopping amplitudes (assumed isotropic in the following of the Section: $w_{\hat{j}} \equiv w$). The phases θ_j depend in general on the position $\mathbf{r}$ and can be thought as the integral of an artificial and classical vector potential $\mathbf{A(r)}$ between neighboring sites:

$$\phi_j(\mathbf{r}) = \int_{\mathbf{r}}^{\mathbf{r}+\hat{j}} \mathbf{A}(\mathbf{x}) \cdot d\mathbf{x}\,. \tag{2}$$

The ladder operators $c_{\mathbf{r}}$ and $c^{\dagger}_{\mathbf{r}}$ annihilate and create an atom in the lattice site $\mathbf{r}$ and they may obey either fermionic or bosonic commutation relations depending on the atoms species.

It is important to emphasize that the artificial vector potential $\mathbf{A}$ constitutes a classical and static field; despite that, we can define $U(1)$ gauge transformations acting on the ladder operators of the previous Hamiltonian and on the vector potentials, which leave the dynamics of the system invariant; $\mathbf{A}$ is thus, in this context, a properly defined gauge potential (see the reviews [20, 32] for more details). Notice as well that one can simulate gauge potentials without a periodic potential [20, 32], but that typically the implementation of magnetic potential in an optical lattice can crucially take advantage of the presence of the lattice potential itself (in other words, decreasing to zero the intensity of the laser beams amounts to make vanishing the magnetic potentials as well).

The effect of the gauge symmetry is that the main observables we must consider are gauge-invariant observables - although, due to the artificial nature of these gauge potentials, also gauge-dependent quantity may be evaluated in the experimental setups, going beyond the previous effective Hamiltonian description. The main gauge-invariant quantity determining the dynamics of the system is the magnetic flux which characterizes each plaquette in the lattice. Such flux describes an

Aharonov-Bohm phase acquired by an atom hopping around a lattice plaquette and can be defined as:

$$\Phi_p = \sum_{(\mathbf{r},\hat{j})\in p} \phi_j(\mathbf{r}) = \oint_p \mathbf{A}(\mathbf{x}) \cdot d\mathbf{x}\,, \tag{3}$$

where $(\mathbf{r},\hat{j})$ labels the links along the plaquette p in order to consider a counterclockwise path. The lattice spacing is denoted by a, and if not differently stated is intended to be set to 1.

On the experimental side there are two broad classes of techniques which have been adopted to engineer effective Hamiltonians of the form in Eq. (1). The first corresponds to the "lattice shaking", which consists in a fast periodic modulation of the optical lattice trapping the atoms whose effect is to reproduce, at the level of the slow motion of the atoms, the required complex hopping amplitudes. The second is the "laser-assisted tunneling" of the atoms in optical lattices in which the atom motion is suppressed along one direction and restored through the introduction of additional Raman lasers able to imprint additional space-dependent phases to the tunneling of the particles. Both these techniques allow for the generation of artificial magnetic fluxes and are based on non-trivial time-dependent Hamiltonians which determine, at the level of the slow motion of the system, a dynamics which can be described by an effective Hamiltonian of the kind in Eq. (1). In the following we will summarize first the technique developed in [31] which provides a very useful tool for the analysis of these driven time-dependent systems, and then we will describe some of the main examples of systems obtained through lattice shaking or laser-assisted tunneling.

2.1 An Effective Description for Periodically Driven Systems

The technique for the analysis of periodically driven systems proposed in [31], whose presentation we follow in this Section, is based on the distinction of two main ingredients whose combination describes the dynamics of modulated setups. The first is an effective Hamiltonian H, independent on the initial conditions of the dynamics, and capturing the long-time motion of the particles in the system. The second is a so-called kick-operator K describing the effects due to the initial and final phases of the modulation. In particular it is responsible for both the initial conditions of the system and for the so-called micro-motion, which includes the periodic dynamics of all the fast-evolving degrees of freedom. To be explicit, let us assume that the modulated system is described by a time-periodic Hamiltonian $\tilde{H}(t) = \tilde{H}(t+T)$. It is then possible to decompose the evolution of the system into:

$$U(t_i \to t_f) = e^{-iK(t_f)} e^{-iH(t_f - t_i)} e^{iK(t_i)}\,. \tag{4}$$

Here H is the effective, time-independent, Hamiltonian, not depending on t_i and t_f; the kick operator $K(t) = K(t+T)$ is a periodic time-dependent operator, and hereafter we set $\hbar = 1$. The approach in [31] consists in a series expansion of H and K in the small parameter $1/\omega = T/(2\pi)$, where ω is the driving frequency of the system and must constitute the largest energy scale of the problem.

To study optical lattices with non-trivial artificial magnetic fluxes it is usually enough to consider the long-term dynamics of the driven system and thus the effective Hamiltonian only (the situation would be different for systems involving also spin degrees of freedom, or for the evaluation of the heating of the driven system). To this purpose, we decompose the time-dependent Hamiltonian $\tilde{H}(t)$ into its Fourier component:

$$\tilde{H}(t) = H_0 + \sum_{n>0} e^{in\omega t} V^{(n)} + \sum_{n>0} e^{-in\omega t} V^{(-n)} \tag{5}$$

with $V^{(-n)} = V^{(n)\dagger}$. H_0 is the time-independent component of $\tilde{H}$, whereas the operators $V^{(-n)}$ are associated to its harmonics. In terms of these operators it is possible to show that the effective Hamiltonian reads:

$$\begin{aligned} H = H_0 &+ \frac{1}{\omega} \sum_{n=1}^{\infty} \frac{1}{n} \left[V^{(n)}, V^{(-n)} \right] + \\ &+ \frac{1}{2\omega^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \left(\left[\left[V^{(n)}, H_0 \right], V^{(-n)} \right] + \text{H.c.} \right) + O(T^3) \,. \end{aligned} \tag{6}$$

This expansion allows for a determination of the effective Hamiltonian in the main examples of systems of ultracold atoms trapped in optical lattices, subject either to a modulation of the trapping lattice or two additional Raman couplings. One needs to consider carefully, though, the issue of the convergence of this series which must be evaluated specifically for each system. The readers are referred to [31] for more detail.

2.2 Artificial Gauge Potentials from Lattice Shaking

The first attempts to experimentally modify the hopping amplitudes of the effective tight-binding models for atoms trapped in optical lattices through the introduction of modulations date back to the works [25, 43, 51]. To understand how the effect of the lattice shaking can determine the tunneling amplitudes of the atoms let us first address a one-dimensional setup. Although, in this case, it is not possible to define magnetic fields and fluxes, the analysis of this simplified system will be useful to understand the appearance of artificial magnetic fluxes in higher dimensions. We consider an optical potential of the form $V(t) = V_0 \sin^2 (x - \xi_0 \cos(\omega t))$ where ω

is the shaking frequency. The Hamiltonian with this oscillating potential can be mapped in a co-moving frame ($x \to x + \xi_0 \cos(\omega t)$) characterized by the following Hamiltonian:

$$\tilde{H}(t) = p^2 + V_0 \sin^2(x) - \frac{1}{2} x \xi_0 \omega^2 \cos(\omega t)\,, \tag{7}$$

where the last term accounts for the additional force in the non-inertial frame and we set the mass to $m = 1/2$ for the sake of simplicity. Finally, by approximating with a tight-binding model we obtain:

$$\tilde{H}(t) = \sum_x \left[-w\, c_{x+1}^\dagger c_x - w\, c_x^\dagger c_{x+1} - \frac{1}{2} x \xi_0 \omega^2 \cos(\omega t) c_x^\dagger c_x \right]. \tag{8}$$

In this case it is possible to derive the full effective Hamiltonian without recurring to a series expansion to obtain [24]:

$$H = -w \mathscr{J}_0(\xi_0 \omega/2) \sum_x c_{x+1}^\dagger c_x + c_x^\dagger c_{x+1} \tag{9}$$

where $\mathscr{J}_0$ is a Bessel function of the first kind which renormalizes the tunneling amplitude and may assume either positive or negative values depending on $\xi_0 \omega$. Despite the fact that, in this case, the hopping amplitude remains always real, it is interesting to notice that it can change sign.

In $1D$ systems, such a change of sign is simply translated in a different dispersion for the single particle problem; however, it is possible to extend this naive example to higher dimensions and less trivial geometries: in this case the result of the lattice shaking provides a first tool for the engineering of non-trivial fluxes. We also observe that, applying the formalism of [31], we have that $H_0 = -w \sum_x c_{x+1}^\dagger c_x +$ H.c., $V^{(1)} = V^{(-1)} = -x\omega^2\, c_x^\dagger c_x/4$ and all the other harmonics are absent. The effective Hamiltonian based on Eq. (6) would then correspond to a series expansion of the Bessel function in Eq. (9) [31].

The lattice shaking techniques can be also extended to obtain complex hopping amplitudes. To this purpose, in this simple one-dimensional model, it is necessary to change the time-dependence of the modulation of the lattice in order to break the time-reversal symmetry [$V(t - t_0) = V(-t - t_0)$] and a shift antisymmetry [$V(t) = V(t + T/2)$] [69]. This has been realized for the first time for a *Rb* Bose-Einstein condensate and the presence of non-trivial hopping phases has been verified through time-of-flight measurements of its momentum distribution as a function of the modulation amplitude [69]. This may be counterintuitive because, in one dimension, the observation of the hopping phase corresponds to the observation of a gauge-dependent quantity. We notice, however, that only the effective tight-binding models adopted in the description of the slow dynamics of the system, and the related observables, are indeed gauge-invariant; in the experiment, though, one can access also additional "gauge-dependent" observables through operations which do not have a physical counterpart in the effective toy model: this is the case of the time-of-flight imaging which follows from switching off the optical lattice. Such procedure maps the crystal momentum of the tight binding model (9) (which is a gauge-dependent quantity) into the velocity of the particles during the time of flight, which is an observable quantity which exists only considering the embedding of the system in the larger laboratory setting.

The effects of lattice shaking become even more remarkable in two-dimensional setups. In this case lattices may be accelerated along two different directions to cause a global periodic motion of the optical lattice around a closed orbit which yields, at the level of the effective Hamiltonian, a tight-binding model with non-trivial fluxes.

On triangular optical lattices this technique has been adopted to realize staggered flux configurations [70] and, more recently, the same method, with a circular modulation of the lattice position [61], has been used to simulate the topological Haldane model [35] on the honeycomb lattice with a gas of fermionic ^{40}K [41]. The Haldane model represents a topological insulator of fermions hopping in a honeycomb lattice with nearest-neighbor and next-nearest-neighbor tunnelings. It is based on both the presence of a pattern of staggered fluxes Φ to break time-reversal symmetry and an onsite staggering potential to break space inversion symmetry [35]. By varying the value of either of these parameters, the model undergoes topological phase transitions, characterized by discontinuities of the Chern number of the lowest energy band. These discontinuities have been experimentally detected through measurements of the drift of the center of mass of the system in the presence of an additional magnetic gradient to add an additional constant force [41].

2.3 Artificial Gauge Potential from Laser-Assisted Tunneling

Complex hopping amplitudes in the effective Hamiltonian can be obtained also through a different technique based on the introduction of pairs of Raman lasers coupling the low-energy states of the atoms trapped in the optical lattice. In this case the phase differences and space dependence of the Raman lasers may be inherited by the dynamics of the atoms, thus allowing for complex space-dependent amplitudes.

To reach this result, however, it is necessary to first suppress the motion of the atoms in the optical lattice, at least, along one direction. This is obtained through the introduction of suitable energy offsets, depending on the positions, which shift the energy of neighboring sites by an energy Δ. These offsets can be obtained, for example, by tilting the lattice (i.e., with gravity), or by introducing suitable magnetic gradients in the system which couple with the atomic magnetic dipole moments (thus generating a position dependent Zeeman term) or through the introduction of superlattices.

Let us start by considering one of the simplest realization of strong fluxes in optical square lattices as experimentally realized [4]. In this experiment an optical superlattice, generated by a standing wave with wavelength $2a$, was used to introduce an additional staggering along the $\hat{x}$ direction for the trapped atoms,

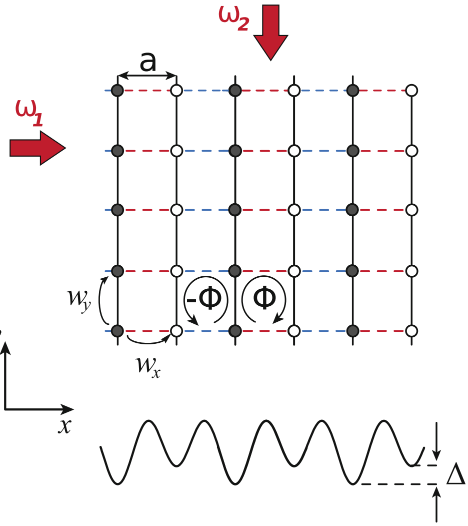

Fig. 1 Schematic illustration of the setup adopted in the experiment [4] for the realization of staggered magnetic fluxes. The tunneling along the horizontal direction is suppressed by the introduction of the staggering Δ through a superlattice. A pair of Raman lasers (*red arrows*) are added to the system to restore the horizontal tunneling. As a result the even horizontal links (*blue dashed links*) acquire a tunneling phase $e^{-i\mathbf{k}_R\mathbf{r}}$, whereas the odd (*red dashed links*) acquire the opposite phase $e^{i\mathbf{k}_R\mathbf{r}}$. $\mathbf{k}_R$ is the recoil momentum of the pair of Raman lasers

such that the initial, time-independent setup can be modeled by the following Hamiltonian:

$$\tilde{H}'_0 = -w \sum_{\mathbf{r},\hat{j}} \left(c^\dagger_{\mathbf{r}+\hat{j}} c_\mathbf{r} + \text{H.c.} \right) + \frac{\Delta}{2} \sum_\mathbf{r} (-1)^x c^\dagger_\mathbf{r} c_\mathbf{r} \tag{10}$$

where $\mathbf{r} = (x, y)$ and Δ is the staggering related to the amplitude of the superlattice (see Fig. 1). Two running Raman lasers with wave vectors $\mathbf{k}_{1,2}$ and frequencies $\omega_{1,2}$, tuned such that $\omega_1 - \omega_2 = \Delta$, are then introduced in the system. The associated electric field is $E_1 \cos(\mathbf{k_1 r} - \omega_1 t) + E_2 \cos(\mathbf{k_2 r} - \omega_2 t)$ which, neglecting the fast oscillating terms, generates a potential:

$$V(t) = \kappa e^{i(\mathbf{k}_R \mathbf{r} - \Delta t)} c^\dagger_\mathbf{r} c_\mathbf{r} + \text{H.c.}, \tag{11}$$

where $\kappa = 2E_1E_2$ and $\mathbf{k}_R = \mathbf{k}_1 - \mathbf{k}_2$ is the recoil momentum of the Raman lasers.

The time-evolution of the system is ruled by the Schrödinger equation $i\partial_t \psi = \tilde{H}'(t)\psi$, where $\tilde{H}'(t) = \tilde{H}'_0 + V(t)$. Since the static Hamiltonian $\tilde{H}'_0$ contains the staggered-potential term that explicitly diverges with the driving frequency Δ, it is convenient to apply the unitary transformation [33, 56]

$$\psi = R(t)\tilde{\psi} = \exp(-iWt)\,\tilde{\psi}, \tag{12}$$

with W being the staggering term:

$$W = \frac{\Delta}{2} \sum_{\mathbf{r}} (-1)^x c_{\mathbf{r}}^\dagger c_{\mathbf{r}} \,. \tag{13}$$

Such transformation removes the diverging term and maps $\tilde{H}'$ into:

$$\tilde{H}(t) = R^\dagger(t) \left[\tilde{H}_0' + V(t)\right] R(t) - W = \tag{14}$$

$$= H_0 + V^{(1)} e^{i\Delta t} + V^{(-1)} e^{-i\Delta t}, \tag{15}$$

where

$$H_0 = -w \sum_{x,y} \left(c_{x,y+1}^\dagger c_{x,y} + c_{x,y}^\dagger c_{x,y+1} \right), \tag{16}$$

$$\hat{V}^{(1)} = \kappa \sum_{\mathbf{r}} e^{-i\mathbf{k}_R \mathbf{r}} c_{\mathbf{r}}^\dagger c_{\mathbf{r}} - w \sum_{x\,\mathrm{odd},y} \left(c_{x+1,y}^\dagger c_{x,y} + c_{x-1,y}^\dagger c_{x,y} \right), \tag{17}$$

$$\hat{V}^{(-1)} = \kappa \sum_{\mathbf{r}} e^{i\mathbf{k}_R \mathbf{r}} c_{\mathbf{r}}^\dagger c_{\mathbf{r}} - w \sum_{x\,\mathrm{even},y} \left(c_{x+1,y}^\dagger c_{x,y} + c_{x-1,y}^\dagger c_{x,y} \right). \tag{18}$$

From these terms it is easy to derive the effective Hamiltonian in Eq. (6) at first order:

$$H = -w \sum_{x,y} \left(c_{x,y+1}^\dagger c_{x,y} + c_{x,y}^\dagger c_{x,y+1} \right) - \tag{19}$$

$$- \frac{w\,\kappa}{\Delta} \sum_{x\,\mathrm{even},y} \left[\left(e^{-i\mathbf{k}_R \hat{x}} - 1 \right) \left(e^{-i\mathbf{k}_R \mathbf{r}} c_{x+1,y}^\dagger c_{x,y} + e^{i\mathbf{k}_R \mathbf{r}} c_{x,y}^\dagger c_{x-1,y} \right) + \mathrm{H.c.} \right] + O(1/\Delta^2)\,,$$

This effective Hamiltonian describes in general a two-dimensional model with staggered magnetic fluxes where the sign of the fluxes alternate in the plaquettes belonging to even and odd columns. In the experiment [4], the recoil momentum was chosen as $\mathbf{k}_R = (\hat{x} + \hat{y})\Phi$. In this case the $\hat{x}$ component has no relevance in the definition of the fluxes and the previous Hamiltonian becomes, after a suitable gauge transformation:

$$H = -w_y \sum_{x,y} \left(c_{x,y+1}^\dagger c_{x,y} + c_{x,y}^\dagger c_{x,y+1} \right) - \tag{20}$$

$$w_x \sum_{x\,\mathrm{even},y} \left[\left(e^{-i\Phi y} c_{x+1,y}^\dagger c_{x,y} + e^{i\Phi y} c_{x,y}^\dagger c_{x-1,y} \right) + \mathrm{H.c.} \right] + O(1/\Delta^2)$$

with $w_y = w$ and $w_x = 2w\kappa \sin(\Phi/2)/\Delta$ (this value is the one obtained at the first order in the perturbative expansion, and it must be considered only an approximation). From the Hamiltonian in Eq. (20) it is evident the alternation of fluxes $\pm\Phi$ on the plaquettes along the horizontal direction.

The introduction of the staggering term, however, allows also for more refined setups in which the even and odd links may be separately addressed [33]. This requires the introduction of two different pairs of Raman lasers with opposite frequency shifts $\pm\Delta$ and it permits to obtain systems with a uniform magnetic flux Φ in each plaquette [33]. In this way the Hofstadter model on the square lattice has been realized for ^{87}Rb [6] and it was possible to measure the Chern number of the different energy bands through the motion of the mass center of the system.

The staggered potential, however, it is not the only possible choice to suppress the motion along one direction. The first quantum simulations with ultracold atoms of the Hofstadter model [5, 60] were instead based on an external potential of the kind $W = \sum_{\mathbf{r}} \Delta x c^{\dagger}_{\mathbf{r}} c_{\mathbf{r}}$. In this case the introduction of two Raman lasers yields indeed to an effective Hamiltonian with rectified fluxes, and this result can be obtained with calculations analogous to the previous one where the distinction between even and odd links is no longer required, and all the horizontal links acquire a tunneling phase of the form $e^{i\mathbf{k}_R\mathbf{r}}$ consistent with a constant flux.

The laser-assisted techniques to design artificial gauge potentials are extremely versatile, and the previous approach can be generalized to different geometries and to multi-component species. The introduction of additional potential through superlattices, for example, enabled the realization of ladder models pierced by uniform fluxes which are characterized by chiral currents and a Meissner-like effect [8]. Furthermore the introduction of spin-dependent potentials, as in [5], permits to mix different spin-species subject to opposite magnetic fluxes and some theoretical proposals generalized these systems to engineer an artificial spin-orbit couplings for two-component atoms [31, 56].

3 Cubic Lattice Tight-Binding Models with Commensurate Flux

In this Section we consider cubic lattices in a magnetic field, focusing on the case of Abelian fluxes. This is a very interesting mathematical problem in itself and it has a counterpart in the experimental implementations we discussed in the previous Section.

3.1 Isotropic Flux

We start our study with a single-species tight-binding model on a cubic lattice with $N = L^3$ sites, in the presence of an Abelian uniform and static magnetic field $\mathbf{B} = \Phi\,(1, 1, 1)$ isotropic on the three directions. This field gives rise on each plaquette of the lattice (with area a^2, a being the lattice spacing) to a magnetic flux $\Phi = \mathbf{B} \cdot \mathbf{a}^2$. The presence of this flux amounts to a phase $e^{i\Phi}$ gathered by a particle hopping around a single plaquette, because of the Stokes theorem. The generalization of this model to many species is straightforward, since an Abelian gauge field does not mix the different species. The magnetic flux is chosen commensurate:

$$\Phi = 2\pi \frac{m}{n} . \tag{21}$$

The commensurate condition allows us to solve the model analytically, imposing periodic boundary condition on the lattice. At variance, in the incommensurate case the determination of spectrum requires a numerical solution of the real space tight-binding matrix, see e.g. [17, 52] - for a discussion of the Hofstadter butterfly in three dimensions see [46], while a study in higher dimensions is reported in [44].

By exploiting the gauge redundancy, the static magnetic field $\mathbf{B}$ can be associated to various physically equivalent gauge potentials $A_\mu(\mathbf{x})$. For the sake of simplicity, we choose here a time-independent gauge configuration, adopting the (static) Coulomb gauge $A_0(\mathbf{x}) = 0$.

Because of the magnetic phases in Eq. (2), the sites of the lattice, all equivalent each other at $\mathbf{B} = 0$, get inequivalent, the inequivalence lying in the phases gathered after each hopping along the bonds starting from a certain site. In this way, the lattice gets divided, in a gauge-dependent way, in a certain number of sublattices. Exploiting this freedom, in order to perform calculations in the easiest way as possible, it is useful to look for the (set of) gauge(s) characterized, for a given commensurate magnetic flux $\Phi = 2\pi \frac{m}{n}$, by the smallest number of sublattices.

A simple (and still not unique) gauge fulfilling this requirement is [37]:

$$\mathbf{A} = \frac{2\pi}{a^2} \frac{m}{n} (0, x - y, y - x) , \tag{22}$$

with permutations in x, y, z also equally acceptable. This gauge is a three-dimensional generalization of the Landau gauge in two dimensions [47], reducing indeed to the Landau gauge in this limit ($w_{\hat{z}} \to 0$), up to a gauge redefinition to absorb the term $-y$ in A_y.

Assuming the choice in Eq. (22), the Hamiltonian in Eq. (1) can be recast in the form

$$H = -\sum_{\mathbf{r}} \left[w_{\hat{x}}\, c^\dagger_{\mathbf{r}+\hat{x}}\, c_{\mathbf{r}} + w_{\hat{y}}\, U_{\hat{y}}(x, y)\, c^\dagger_{\mathbf{r}+\hat{y}} c_{\mathbf{r}} + w_{\hat{z}}\, U_{\hat{z}}(x, y)\, c^\dagger_{\mathbf{r}+\hat{z}} c_{\mathbf{r}} \right] + \text{H.c.} , \tag{23}$$

where the tunneling magnetic phases $U_{\hat{j}}(x, y) = e^{i\,\phi_{\hat{j}}(x,y)}$ are defined as:

$$U_x = 1 , \tag{24}$$

$$U_{\hat{y}}(x, y) = \exp\left(i \int_{x,y,z}^{x,y+a,z} A_y\, \mathrm{d}y\right) = \exp\left(i\, 2\pi \left(\frac{x-y}{a} - \frac{1}{2}\right) \frac{m}{n}\right) , \tag{25}$$

$$U_{\hat{z}}(x, y) = \exp\left(i \int_{x,y,z}^{x,y,z+a} A_z\, \mathrm{d}z\right) = \exp\left(-i\, 2\pi \left(\frac{x-y}{a}\right) \frac{m}{n}\right) . \tag{26}$$

The hopping phases in Eqs. (25) and (26) explicitly depend on the positions labelled modulo n. Since the z coordinate is not present in Eq. (22), every wave-function of the Hamiltonian in Eq. (23) can be written as [50]:

$$\psi(x, y, z) = e^{ik_z z} u(x, y) , \tag{27}$$

allowing for a dimensional reduction of the eigenvalues problem as for the corresponding problem in two dimensions where the Harper equation is found [38, 71].

The Hamiltonian in Eq. (23) with the hopping phases in Eqs. (24)–(26) is translational invariant. For gauge invariant systems, translational invariance implies that a translation of the coordinates by a vector $\mathbf{w}$ transforms the Hamiltonian of the system to a gauge-equivalent one [50], and one may find [49]:

$$H(\mathbf{r} + \mathbf{w}) = \mathscr{T}_{\mathbf{w}}^{\dagger}(\mathbf{r}) H(\mathbf{r}) \mathscr{T}_{\mathbf{w}}(\mathbf{r}) , \tag{28}$$

with $\mathscr{T}_{\mathbf{w}}(\mathbf{r}) \in U(1)$ being a suitably chosen local gauge transformation which depends on $\mathbf{w}$.

The Hamiltonian in Eq. (23) with the gauge potential in Eq. (22) is translationally invariant because it fulfills Eq. (28). We stress that the potentials of the form in Eq. (22) are not the only ones satisfying the condition in Eq. (28), but instead all the potentials obtained from Eq. (22) through local gauge transformation are characterized by the same physical translational invariance. The property in Eq. (28) is indeed a physical property of the system which is reflected on all the gauge-invariant observables, as for example, the Wilson loops $W(\mathscr{C}) = \mathbf{P} e^{i \oint_{\mathscr{C}} \mathbf{A}(\mathbf{r}) \cdot d\mathbf{r}}$ evaluated on closed paths along the lattice.

The Hamiltonian in Eq. (23) is also periodic with period n along $\hat{x}$ $\hat{y}$, due to the presence of the nontrivial magnetic hopping phases $U_{\hat{y}}(x, y)$, $U_{\hat{z}}(x, y)$, thus the reduced wavefunctions $u(x, y)$ have the same periodicity. In this way the magnetic unitary cell, defined by the elementary translations leading from a site to equivalent ones in the three lattice directions, can be defined now as enlarged n times along two directions (say $\hat{x}, \hat{y}$).

The problem to find the eigenvalues of the Hamiltonian in Eq. (23) on a lattice with N number of sites would naïvely require in general the diagonalization of a $N \times N$ adjacency matrix in real space. However, assuming translational invariance, the calculation can be remarkably simplified by exploiting the division in sublattices seen above. Indeed, in the presence of a magnetic flux $\Phi = 2\pi \frac{m}{n}$ and working in the gauge in Eq. (22), the cubic lattice divides in n sublattices, labelled by the quantity $(x - y)\,\mathrm{mod}(n)$. In this way the Hamiltonian in Eq. (23) becomes:

$$H = -\sum_{\hat{j}} w_{\hat{j}} \sum_{s} e^{i\phi_{s\hat{j}}} \sum_{\mathbf{r}_s} c^{\dagger}_{\mathbf{r}_s + \hat{j}} c_{\mathbf{r}_s} + \text{H.c.} , \tag{29}$$

where s labels the sublattices and $\mathbf{r}_s$ labels the sites of the s-th sublattice.

Since the magnetic unitary cell is defined now as enlarged n times along two directions, the corresponding magnetic Brillouin zone (MBZ) in momentum space becomes $\{\frac{2\pi}{a}, \frac{2\pi}{an}, \frac{2\pi}{na}\}$ [or other permutations of the factors $\frac{1}{n}$ between the space directions, consisting in a mere redefinition of $\mathbf{A}(\mathbf{r})$]. Correspondingly, the allowed momenta $\mathbf{k}$ are $\frac{N}{n^2}$, of the form $\mathbf{k} = \{\frac{2\pi}{aL_x}p_x, \frac{2\pi}{aL_y}p_y, \frac{2\pi}{aL_z}p_z\}$, with $p_{\hat{x}} = 0, \ldots, L-1$ and $p_{\hat{y},\hat{z}} = 0, \ldots, \frac{L}{n} - 1$. In this way, all the physical quantities display a momentum periodicity $\mathbf{k} \to \mathbf{k} + \frac{2\pi}{na}(l_x, l_y, l_z)$, with l_i being again integer numbers.

The counting of the $\frac{N}{n^2}$ allowed momenta proceeds as follows: each sublattice differs from another one by $\pm\hat{x}$ or $\pm\hat{y}$ translations that are not primary, then we correspondingly expect n sets of $\frac{N}{n}$ inequivalent energy eigenstates [50]. These sets form n subbands in the MBZ. However, any sublattice is further divided in n sub-sublattices differing by a primary translation $\pm(\hat{x} + \hat{y})$, leaving invariant the potential in Eq. (22). In this way, any $\frac{N}{n}$-fold set of eigenstates is again partitioned in n equivalent and degenerate sub-sets, each one having $\frac{N}{n^2}$ element. These elements are parametrized by the $\frac{N}{n^2}$ momenta in the MBZ described above. Moreover the second partition translates in n-fold degeneracy of each subband. In the particular case $\Phi = \pi$, two sub-bands are obtained, touching in Weyl cones as discussed in [23, 48, 49]; in this case the system in Eq. (23) is the direct three-dimensional generalization of the square lattice model with π-fluxes in [1].

The Hamiltonian in Eq. (29) can be expressed in momentum space using the formulas $c_{\mathbf{r}_s} = \frac{1}{\sqrt{N/n^2}} \sum_{\mathbf{k}} c(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{r}_s}$ and $\sum'_{\mathbf{r}_s} e^{i\mathbf{k}\cdot\mathbf{r}_s} = \frac{N}{n^2}$. The vectorial label $\mathbf{r}_s$ runs here on the $\frac{N}{n^2}$ sites of one sub-sublattice of the sublattice s, the upper index in the sum of the second formula meaning this restriction. We obtain:

$$H = -\sum_{\mathbf{k}} \sum_{\hat{j}} w_{\hat{j}} \sum_{s} e^{i\phi_{s\hat{j}}}\, e^{-i\mathbf{k}\cdot\mathbf{j}}\, c^{\dagger}_{s'=s+\hat{j}}(\mathbf{k})\, c_s(\mathbf{k}) \; + \text{H.c.}\,, \tag{30}$$

where we have also taken into account that, starting from the s-th sublattices and moving in the $\hat{j}$ direction, a new sublattice (denoted as s') is univocally found, as consequences of Eq. (22). This is the reason oh the notation $s' = s + \hat{j}$.

The Hamiltonian in Eq. (30) can be recast in the sublattices basis as:

$$H = -\sum_{\mathbf{k}} \sum_{\hat{j}} w_{\hat{j}} \sum_{s} c^{\dagger}_{s'=s+\hat{j}}(\mathbf{k}) \left(T^{\mathrm{AB}}_{\hat{j}}\right)_{s',s} e^{-i\mathbf{k}\cdot\mathbf{j}}\, c_s(\mathbf{k}) \; + \; \text{H. c.}\,, \tag{31}$$

where $T^{\mathrm{AB}}_{\hat{j}}$ are $n \times n$ hopping matrices in the sublattice basis, reading, up to ciclic permutations $\mathbf{Z}_n$:

$$T^{\mathrm{AB}}_{\hat{x}} = \begin{pmatrix} 0 \; 1 \ldots 0 \\ 0 \; 0 \; \ddots \; 0 \\ 0 \; 0 \ldots 1 \\ 1 \; 0 \;\; 0 \;\; 0 \end{pmatrix} T^{\mathrm{AB}}_{\hat{y}} = e^{-i\pi\frac{m}{n}} \begin{pmatrix} 0 & \ldots & 0 & \varphi_0 \\ \varphi_1 & 0 & \ldots & 0 \\ 0 & \ddots & 0 & 0 \\ 0 & \ldots & \varphi_{n-1} & 0 \end{pmatrix} T^{\mathrm{AB}}_{\hat{z}} = \begin{pmatrix} \varphi_0 & 0 & \ldots & 0 \\ 0 & \varphi_{n-1} & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & \ldots & \varphi_1 \end{pmatrix}, \tag{32}$$

with $\varphi_l = e^{i2\pi \frac{m}{n} l}$, $l = 0, \ldots, n-1$.

The matrices $T^{\text{AB}}_{x,\hat{y},z}$ do not commute each other, implying that the unitary cell of the lattice does not coincides with its geometric smallest cell (with area a^2), as seen above. However, the n-power of these matrices yields the identity: $\left(T^{\text{AB}}_{\{\hat{x},\hat{y},\hat{z}\}}\right)^n = \mathbf{1}_{n\times n}$, recovering the MBZ $\{\frac{2\pi}{a}, \frac{2\pi}{an}, \frac{2\pi}{an}\}$. Moreover, if $\frac{m}{n} \neq \frac{1}{2}$ the unitary matrices $T^{\text{AB}}_{x,\hat{y},z}$ are not invariant (even possibly up to a global phase) by the conjugate operation, reflecting the breaking of the time-reversal symmetry, due to the magnetic field $\mathbf{B}$ itself. A notable result of the discussion above is that the diagonalization of a $N \times N$ matrix is reduced to the diagonalization of a $n \times n$ one.

We conclude this Section by observing that in the presence of more species (labelled by the index $\alpha = 1, \ldots, m$) hopping on the lattice and subject to the Abelian gauge potential in Eq. (22), the Hamiltonian in Eq. (31) generalizes to

$$H = -\sum_{\mathbf{k}} \sum_{\hat{j}} w_{\hat{j}} \sum_{s} c^{\dagger}_{s'=s+\hat{j},\alpha'}(\mathbf{k}) \left(T^{\text{AB}}_{\hat{j}} \otimes \mathbf{1}_{m\times m}\right)_{s',\alpha',s,\alpha} e^{-i\mathbf{k}\cdot\mathbf{j}}\, c_{s,\alpha}(\mathbf{k}) + \text{H. c.}, \tag{33}$$

where no mixing of the different species involved occurs.

3.2 Generalization: Anisotropic Abelian Lattice Fluxes

In the previous analysis we assumed that the value of the fluxes was the same for the three orientations of the plaquettes. Now we discuss some extension in which we relax this hypothesis. We analyze first the case in which the magnetic field $\hat{z}$ is perturbed, such that we introduce an anisotropy in the previous system:

$$\mathbf{B} = \frac{2\pi}{a^2}\left(\frac{m}{n}, \frac{m}{n}, \frac{m_z}{n_z}\right). \tag{34}$$

Again we may assume, without any loss of generality, m_z and n_z prime with each other as well as m and n. In the case of Eq. (34), a gauge similar to the one in Eq. (22) can be used:

$$\mathbf{A} = \frac{2\pi}{a^2}\left(0, \frac{m_z}{n_z}(x-y), \frac{m}{n}(y-x)\right). \tag{35}$$

This choice still depends on one parameter only, thus ensuring the appearance of minimal gauge-dependent sublattices. More in detail, the lattice divides again in $n_2 = \text{l. c. m.}\,(n, n_z)$ inequivalent sublattices, defined by the periodicity of the phases in the $\hat{x}$ and $\hat{y}$ directions and labelled by the set $(x-y)\text{mod}(n_2)$. Indeed the hopping phases from Eq. (35) are:

$$\phi_{\mathbf{r}+\hat{j},\mathbf{r}} = \frac{2\pi}{a}\left(0, \frac{m_z}{n_z}\left(x-y-\frac{a}{2}\right), \frac{m}{n}(y-x)\right). \tag{36}$$

Similarly to the previous case, each sublattice is again divided in n_2 equivalent subsublattices, each one having $\frac{N}{n_2^2}$ sites. For this reason, similarly to the Sect. 3.1, n_2 subbands appear, each of them with a n_2 degeneracy. Correspondingly the BZ divides by n_2 in two directions, so that $\mathbf{k} = \{\frac{2\pi}{aL_x} p_x, \frac{2\pi}{aL_y} p_y, \frac{2\pi}{aL_z} p_z\}, p_{\hat{x}} = 0, \ldots, L-1$, $p_{\hat{y},\hat{z}} = 0, \ldots, \frac{L}{n_2} - 1$, or permutations in the pairs of the restricted momentum directions. The Hamiltonian in Eq. (1) can then be rewritten, in terms of these quasi-momenta, as in Eq. (31), by means of three $m_2 \times m_2$ matrices in the basis of the m_2 sublattices, derived similarly to the ones in Eq. (32).

In the completely asymmetric case the magnetic potential reads

$$\mathbf{B} = \frac{2\pi}{a^2}\left(\frac{m_x}{n_x}, \frac{m_y}{n_y}, \frac{m_z}{n_z}\right), \tag{37}$$

a convenient gauge choice, inducing the magnetic field in Eq. (37), reads:

$$\mathbf{A_{AB}} = \frac{2\pi}{a^2}\left(\left(\frac{m_y}{n_y} - \frac{m_x}{n_x}\right)(z-x), \frac{m_z}{n_z}(x-y), \frac{m_x}{n_x}(y-x)\right). \tag{38}$$

The hopping phases from Eq. (38) are:

$$\phi_{\mathbf{r}+\hat{j},\mathbf{r}} = \frac{2\pi}{a}\left(\left(\frac{m_y}{n_y} - \frac{m_x}{n_x}\right)\left(z - x - \frac{a}{2}\right), \frac{m_z}{n_z}\left(x - y - \frac{a}{2}\right), \frac{m_x}{n_x}(y-x)\right). \tag{39}$$

The gauge in Eq. (38), similarly to the previous case, ensures the appearance of the minimum number of gauge-dependent sublattices. In particular, due to the simultaneous x dependence of all the components of $\mathbf{A}_{\mathrm{AB}}$ and following the same logic as in the Sect. 3.1, we obtain

$$n_s = \text{l. c. m. } (n_x, n_y, n_z) \tag{40}$$

inequivalent sublattices (obtained varying y and z at fixed x) and corresponding subbands. Again each sublattice is then further divided in equivalent subsublattices.

More in detail, the counting of these subsublattices proceeds as follows. Starting from a point (x_0, y_0, z_0) belonging to a certain sublattice, they are obtained by adding 1 to each components: $(x_0, y_0, z_0) \to (x_0 + 1, y_0 + 1, z_0 + 1)$. The variable z has periodicity given by l. c. m. (n_x, n_y) possible inequivalent values, y has periodicity l. c. m. (n_x, n_z) and finally x has l. c. m. (n_x, n_y, n_z) inequivalent values. For this reason each inequivalent sublattice divides in

$$\begin{aligned} n_d &= \min\Big(\text{l. c. m. } (n_x, n_y), \text{l. c. m. } (n_x, n_z), \text{l. c. m. } (n_x, n_y, n_z)\Big) = \\ &= \min\Big(\text{l. c. m. } (n_x, n_y), \text{l. c. m. } (n_x, n_z)\Big) \end{aligned} \tag{41}$$

equivalent subsublattices.

Correspondingly, we find $\frac{N}{n_s \times n_d}$ quasi-momenta defining each subband: $\mathbf{k} = \{\frac{2\pi}{aL_x} p_x, \frac{2\pi}{aL_y} p_y, \frac{2\pi}{aL_z} p_z\}$, $p_{\hat{x}} = 0, \ldots, L-1$, $p_{\hat{y}} = 0, \ldots, \frac{L}{n_s} - 1$, $p_{\hat{z}} = 0, \ldots, \frac{L}{n_d} - 1$, or permutations in the pairs of the restricted momentum directions. The Hamiltonian in Eq. (1) can be then rewritten, in terms of these quasi-momenta and in the basis of the n_s sublattices as in Eq. (31), by means of three $n_s \times n_s$ matrices similar to the ones in Eq. (32).

4 Two Applications of Synthetic Gauge Potentials in 1*D* Rings

The possibilities offered by ultracold atoms in optical lattices to engineer tight-binding models in tunable magnetic potential open as well new possibilities also in the field of quantum information in the sense that they could be used in perspective to perform quantum information tasks and control the amount of entanglement of the system. Here, as two examples we believe paradigmatic of such potentialities, we want to shortly address two specific applications showing how tuning a gauge potential could modify the capability of a system to share quantum information. We consider one-dimensional models of free fermions on a ring geometry in the presence of a synthetic magnetic field piercing the ring. We first analyze for short-range lattice models how a topological phase helps to enhance the fidelity in a quantum state transfer (QST) process between different sites of the lattice [7, 62]. Then we study a long-range model to see how the presence of a topological phase can lead to the a volume-law behavior of the entanglement entropy (EE) for the ground state of the system.

4.1 Quantum State Transfer in a Ring Pierced by a Magnetic Flux

We consider a one-dimensional tight-binding model for free fermions with nearest-neighbors hopping in a ring geometry embedded in a magnetic field. Such magnetic field determines the boundary conditions of the problem: its role is to induce an Aharonov-Bohm phase in the transport of a particle along a full circle around the ring geometry. The Hamiltonian of the system reads

$$H = -w \sum_j e^{i\phi} c_j^\dagger c_{j+1} + h.c., \tag{42}$$

where $\phi = \frac{2\pi}{N_S} \Phi$ (Φ being the Abelian magnetic flux piercing the ring chain in units of 2π), N_S is the number of sites, and the site coordinate is $r = aj \bmod N_S$.

The single-particle energy dispersion is

$$E_k(\phi) = -2w\cos(ak-\phi) = 2t\cos\left(\frac{2\pi}{N_S}(n_k-\Phi)\right) , \tag{43}$$

with $k = \frac{2\pi}{aN_S} n_k$. Due to the nontrivial phase $e^{i\phi}$, the single-particle dispersion is shifted, as well as the points corresponding to the Fermi surface. For a single fermion, the introduction of this topological phase affects the wave-packet diffusion, giving a useful tool to optimize the quantum state transfer of a certain state from a part of the chain to another one.

One can consider a fermion initially localized at the time $t = 0$ around the site $j = 0$:

$$|\psi_0(0)\rangle = \sum_j g_j c_j^\dagger |0\rangle , \tag{44}$$

with a square wave packet distribution extended over $\lambda = 2M + 1$ sites:

$$g_l = \begin{cases} \frac{1}{\sqrt{2M+1}} & \text{If } -M \le l \le M \\ 0 & \text{elsewhere} . \end{cases} \tag{45}$$

After the state evolution $|\psi_0(t)\rangle = e^{-iHt}|\psi_0(0)\rangle$, the capacity for the channel to produce QST from the site $j = 0$ to site $j = d$ can be measured by the square projection of the evolved state on the initial state localized on the site d:

$$F_d(t) = |\langle\psi_d(0)|\psi_0(t)\rangle|^2 \simeq A(t)\, e^{-\frac{[d+2wt\sin\phi]^2}{2\sigma_F^2(t)}} , \tag{46}$$

with

$$A(t) = \frac{3\lambda^2}{\pi\sqrt{(\lambda^2-1)^2 + 144w^2t^2\cos^2\phi}} , \tag{47}$$

and

$$\sigma_F^2(t) = \frac{(\lambda^2-1)^2 + 144w^2t^2\cos^2\phi}{12(\lambda^2-1)} . \tag{48}$$

For $\phi = -\pi/2$, the dispersion becomes approximately linear and the wave-packet does not diffuse. Moreover, it propagates with velocity $v = 2w$ causing an enhancement in the fidelity (see Fig. 2). In particular, $F_d(t)$ assumes its maximum value at the approximate time

$$t^* = \frac{d}{2w}. \tag{49}$$

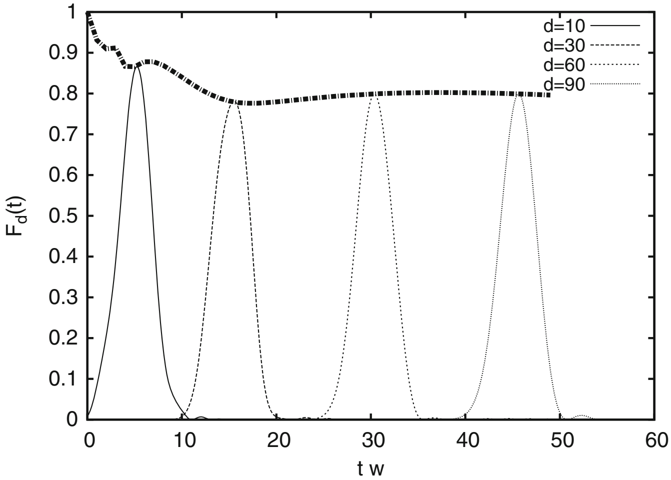

Fig. 2 Time evolution of the fidelity $F_d(t)$ in the square packet preparation ($M = 5$), with phase $\phi = -\pi/2$, different values for the final site $d = 10, 30, 60, 90$ and $N = 500$. The *thick line* indicates the maxima of fidelity reached by each site at different times

4.2 Violation of the Area-Law in Long-Range Systems

The study of the ground-state entanglement properties plays an essential role in the characterization of a quantum many-body system. In this Section, we show how the introduction of a gauge potential in a free-fermion model with a long-range hopping can qualitatively change the scaling behavior of the ground state entanglement. The amount of entanglement of a pure state is well quantified by the so-called Entanglement Entropy (EE), defined as follows. Partitioning a given system in two subsystems A and its complement $\bar{A}$, the EE is the Von Neumann entropy S of one of the two subsystems (say A) calculated from its reduced density matrix ρ_A:

$$S = -Tr\left(\rho_A \ln \rho_A\right) \ . \tag{50}$$

Typically for gapped short-range quantum systems (where gapped means with a finite energy difference of the first excited level, compared to the ground state energy), the EE grows as the boundary of the subsystem A, i.e., for a system in d dimensions the EE scales as $S \propto \partial L^{d-1}$. This is commonly known as the *area law* [26]. The physical origin of this law is that entanglement is appreciably nonvanishing only between parts of the system very close each others, since the quantum correlation functions between two points decay exponentially with their distance, with a finite decay constant ξ that increases as the mass gap decreases. At variance, for short-range free fermionic systems at a critical (gapless) point it has been shown that the divergence of ξ (resulting in an algebraic decay of quantum correlations) produces a logarithmic correction of the area law, $S \propto L^{d-1} \ln L$ [30, 76], so that in one dimension one expects to find $S \propto \ln L$. A more relevant, non-logarithmic, violation of the area law is obtained when $S \propto L^{\beta}$ with $d-1 < \beta < d$. When $\beta = d$ one has a *volume law*.

Referring to free fermions on a lattice, in order to find violation to the area law in gapped regimes, one has to introduce longer-range connections, changing the Fermi surface in a suitable way. In one-dimensional short-range systems, the Fermi surface is typically composed by a finite set of points. This is what happens also in the simplest long-range models when, despite of the long-range hoppings, strong entanglement is created only between closed lattice sites. At variance, if the Fermi surface is a set of points with finite dimension, it can occurs that antipodal sites of the lattice becomes maximally entangled (Bell pairs). As a consequence, a bipartition into two connected complementary parts would cut a number of Bell pairs of the order of the volume of the smaller subsystem, giving rise to a violation of the area law. To this aim, a long-range connection appears useful but not sufficient.

A possible way to create a nontrivial Fermi surface is to introduce a gauge potential [34]. Let us consider a model with long-range hopping with periodic boundary conditions:

$$H = -\sum_{j} w_{i,j} c_i^{\dagger} c_j + h.c. \tag{51}$$

with

$$w_{i,j} = w \frac{e^{i\,\phi\, d_{i,j}}}{|d_{i,j}|^{\alpha}}, \tag{52}$$

where $\phi = \frac{2\pi}{N_S}\Phi$, being Φ a constant, N_S the number of sites. The filling f is defined to be $f = N/N_S$, where N is the number of sites. $d_{i,j}$ is the oriented distance between the sites i and j,

$$d_{i,j} = \begin{cases} (i-j) & \text{if } |i-j| \leq N_S - |i-j| \\ -N_S + |i-j| & \text{otherwise.} \end{cases} \tag{53}$$

Due to the translational invariance, the eigenstates are plane waves, and, for finite N_S, the spectrum is given by:

$$E_k = -2w \begin{cases} \sum_{m=1}^{\frac{N-1}{2}} \frac{1}{m^{\alpha}} \cos\left((k+\phi)m\right) & \text{for odd } N_S\,, \\ \sum_{m=1}^{\frac{N}{2}-1} \frac{1}{j^{\alpha}} \cos\left((k+\phi)\,m\right) + \frac{\cos(\pi n_k)}{2\left(\frac{N_S}{2}\right)^{\alpha}} & \text{for even } N_S\,. \end{cases} \tag{54}$$

For $\phi = 0$, the single-particle spectrum is always monotonous in the interval $k \in [0, \pi]$, while for $\phi \neq 0$ the spectrum can split in two branches for $\alpha < \alpha_c < 1$,

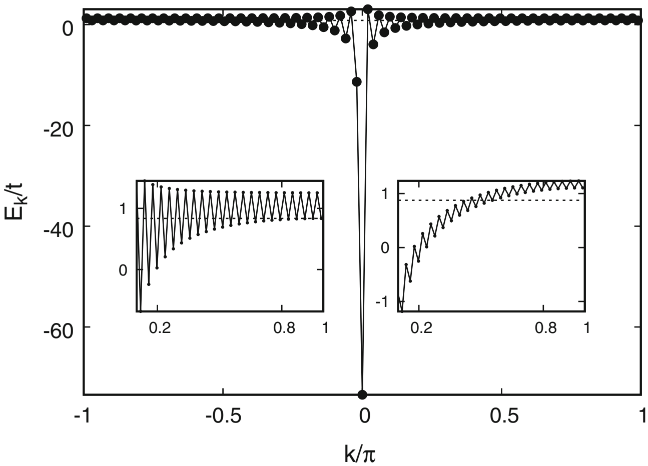

Fig. 3 Spectrum of the Hamiltonian in Eq. (51) with $\Phi = 0.1$, $\alpha = 0.1$, filling factor $f = 0.5$ and $N_S = 100$. *Left inset*: detail of the main plot showing the alternating occupation of the modes k, the Fermi energy corresponding to the *dashed line*. *Right inset*: decrease of the alternating occupation with increasing α. We set $\Phi = 0.1$, $\alpha = 0.4$, $f = 0.5$ and $N_S = 100$

where the critical value α_c depends both on N and ϕ. This means that at fixed ϕ and $N_S \gg 1$ at half-filling, all the momenta k are occupied in an alternating way, as shown in Fig. 3. Thus, for $\alpha < \alpha_c$ and at half-filling, the ground-state is a Bell-paired state, and the EE grows linearly with N_s (with slope $\ln 2$), resulting in a volume law and the Fermi surface has a fractal counting box dimension $d_{box} = 1$. On the contrary, when $\alpha > \alpha_c$ only a fraction of the momenta are occupied in an alternating way, since the "zig-zag" structure of the dispersion relation is partially lost. As a result, the slope of the EE decreases.

We conclude by observing that as long as the dispersion is such that the half-filling occupation is alternate in k, entanglement is created between antipodal sites and the system violates the area law behavior, in favour of a volume law.

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Relative-Zeta and Casimir Energy for a Semitransparent Hyperplane Selecting Transverse Modes

Claudio Cacciapuoti, Davide Fermi, and Andrea Posilicano

Abstract We study the relative zeta function for the couple of operators A_0 and A_α, where A_0 is the free unconstrained Laplacian in $L^2(\mathbf{R}^d)$ $(d \geq 2)$ and A_α is the singular perturbation of A_0 associated to the presence of a delta interaction supported by a hyperplane. In our setting the operatorial parameter α, which is related to the strength of the perturbation, is of the kind $\alpha = \alpha(-\Delta_\parallel)$, where $-\Delta_\parallel$ is the free Laplacian in $L^2(\mathbf{R}^{d-1})$. Thus α may depend on the components of the wave vector parallel to the hyperplane; in this sense A_α describes a semitransparent hyperplane selecting transverse modes.

As an application we give an expression for the associated thermal Casimir energy. Whenever $\alpha = \chi_I(-\Delta_\parallel)$, where χ_I is the characteristic function of an interval I, the thermal Casimir energy can be explicitly computed.

Keywords Casimir effect • Delta-interactions • Finite temperature quantum fields • Relative zeta function • Zeta regularization

MSC 2010 81Q10, 81T55, 81T10

1 Introduction

Analytic continuation techniques are well known to be useful to give a meaning to otherwise divergent series. The most classical example is the Riemann zeta function. The series

$$\zeta^R(s) := \sum_{n=1}^{\infty} \frac{1}{n^s} \tag{1}$$

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A. Michelangeli, G. Dell'Antonio (eds.), *Advances in Quantum Mechanics*, Springer INdAM Series 18, DOI 10.1007/978-3-319-58904-6_5

converges only for $s \in \mathbf{C}$ with Re $s > 1$; however, it is well known that the function $s \mapsto \zeta^R(s)$ can be analytically continued to all complex $s \neq 1$. In this way one can formally evaluate the series in Eq. (1) also for Re $s < 1$.

The same regularization procedure can be used to give a meaning to divergent series arising when computing traces of powers of operators, such as Tr A^{-s}. Indeed, when A is a positive, elliptic differential operator with pure point spectrum, which we denote by $\{\lambda_n\}_{n=1}^{\infty}$ ($\lambda_n > 0$ and each eigenvalue is counted with its multiplicity), one can set, in analogy with Eq. (1),

$$\zeta(A; s) := \mathrm{Tr}\, A^{-s} = \sum_{n=1}^{\infty} \frac{1}{\lambda_n^s} \,. \tag{2}$$

The striking feature of the function $\zeta(A; s)$ is that, even though the series on the r.h.s. converges only for large enough Re s, under certain assumptions on the operator A it can be extended to a meromorphic function with possible poles only on the real line, see [34].

When the essential spectrum of the operator A is not empty the regularization procedure described above cannot be applied. This is the case, for example, when the operator A is the Laplacian on a non compact manifold; in such a situation the trace Tr A^{-s} cannot be defined for any $s \in \mathbb{C}$.

Zeta-regularization techniques, however, turn out to be a powerful tool also in these circumstances if one is interested in the comparison between two operators: an operator A associated to the "interacting" dynamics and a reference "non interacting" or "free" operator A_0. Both A and A_0 are assumed to be nonnegative, they may have non empty essential spectrum and the traces Tr A^{-s} and Tr A_0^{-s} may not be defined. Nevertheless, what may be defined is the *relative zeta function* $\zeta(A, A_0; s) := \mathrm{Tr}\,(A^{-s} - A_0^{-s})$.

In certain situations the relative zeta function can be equivalently expressed in terms of the heat semigroups. We recall the following result from [36]. If the operator $(A - z)^{-1} - (A_0 - z)^{-1}$, with z in the resolvent set of A and A_0, is trace class, and such trace has certain asymptotic expansions for $z \to 0$ and $z \to \infty$ (see [36] and [29] for the details), then the formula

$$\zeta(A, A_0; s) = \frac{1}{\Gamma(s)} \int_0^{\infty} t^{s-1}\, \mathrm{Tr}\,(e^{-tA} - e^{-tA_0})dt \tag{3}$$

holds true for $s_0 \leq \mathrm{Re}\, s \leq s_1$, with s_0 and s_1 depending on the asymptotic expansions of the trace, and where $\Gamma(s)$ is the Gamma function.

The subject of our paper is the study of the relative zeta function for the couple of operators A_0 and A_α defined as follows (see Sect. 2 for the rigorous definitions):

- A_0 is the free unconstrained Laplacian in $L^2(\mathbf{R}^d)$ $(d \geq 2)$.
- A_α is the Laplacian in the presence of a semitransparent hyperplane selecting transverse modes. More precisely, let π denote the hyperplane

$$\pi := \{\mathbf{x} \in \mathbf{R}^d \,|\, x^1 = 0\}\,; \tag{4}$$

this is naturally identified with $\mathbf{R}^{d-1}$. A_α is the self-adjoint operator in $L^2(\mathbf{R}^d)$ which formally corresponds to the Laplacian plus a singular potential supported by the hyperplane π. In our setting the parameter α, which is related to the "strength" of the potential, may depend on the components of the wave vector parallel to π. More precisely, we set $\alpha = \alpha(-\Delta_\parallel)$, where $-\Delta_\parallel$ is the free unconstrained Laplacian in $L^2(\mathbf{R}^{d-1})$. Heuristically speaking, this indicates that the singular potential supported on π acts differently, depending on the transverse modes (parallel to the hyperplane). Denoting by δ_1 the 1-dimensional Dirac delta in $x^1 = 0$, the operator A_α formally corresponds to the heuristic expression "$A_\alpha = -\Delta + \langle \delta_1, \cdot \rangle\, \delta_1 \otimes \alpha(-\Delta_\parallel)$" on $L^2(\mathbf{R}^d) \equiv L^2(\mathbf{R}) \otimes L^2(\mathbf{R}^{d-1})$.

We remark that both operators, A_α and A_0, enjoy the translation invariance in the directions $\mathbf{x}_\parallel$ parallel to π. This symmetry of the system has two important consequences. On one side the operator $A_\alpha^{-s} - A_0^{-s}$ is not trace class no matter how large Re s is (a similar remark holds true for the operator $e^{-tA_\alpha} - e^{-tA_0}$). On the other hand it is clear that any relevant (possibly infinite) physical quantity cannot depend on the coordinate $\mathbf{x}_\parallel$ and can be associated to a finite density by averaging on any finite subset of π. With this remark in mind, and by Eq. (3), we infer that the quantity of interest in our analysis is the relative zeta function

$$\zeta_1(s) \equiv \zeta_1(A_\alpha, A_0; s) := \frac{1}{\Gamma(s)} \int_0^{+\infty} dt\, t^{s-1} \int_{\mathbf{R}} dx^1\, \mathscr{Q}^{rel}(t; x^1, x^1, \mathbf{0}) \,, \tag{5}$$

where $\mathscr{Q}^{rel}(t; x^1, y^1, \mathbf{x}_\parallel - \mathbf{y}_\parallel)$ is the integral kernel of the operator $Q^{rel}(t) := e^{-tA_\alpha} - e^{-tA_0}$. We remark that here we have used the translation invariance of the system to conclude that the integral kernel $\mathscr{Q}^{rel}$ is a function of $\mathbf{x}_\parallel - \mathbf{y}_\parallel$.

We also note that the integrand function in Eq. (5) has been obtained by taking $x^1 = y^1$ and $\mathbf{x}_\parallel = \mathbf{y}_\parallel$ in the integral kernel $\mathscr{Q}^{rel}(t; x^1, y^1, \mathbf{x}_\parallel - \mathbf{y}_\parallel)$. Since the integrand function does not depend on $\mathbf{x}_\parallel$, the integral $\int_{\mathbf{R}} dx^1$ could be rewritten in terms of the average $|\Omega|^{-1} \int_{\mathbf{R}} dx^1 \int_\Omega d\mathbf{x}_\parallel$, where Ω is any finite region of π of volume $|\Omega|$. In this way, taking the limit $\Omega \to \mathbf{R}^{d-1}$, would reconstruct an "averaged trace" of the operator $Q^{rel}(t)$. In the applications, for example when computing the thermal Casimir energy (see Sect. 4), the "average argument" could be made rigorous. A possible approach would be to constrain the system to a rectangular box of size L along the directions $\mathbf{x}_\parallel$, take the average with respect to the volume of the box, and then take the limit $L \to \infty$. Here we do not pursue this goal, we just recall that the problem of the reduction to a density was already present in the original paper by Casimir [7] as well as in more recent papers such as [22]. In the latter work this problem is approached by adding a mass parameter that afterwords is sent to infinity.

Our main result is summed up in Eqs. (41)–(43), where we give the analytic continuation of the map $s \to \zeta_1(s)$.

As an application, in Sect. 4, we compute the thermal Casimir energy per unit surface for a massless scalar field at temperature $T = 2\pi/\beta$, and discuss an explicit choice of the function α.

In the remaining part of the introduction we discuss the physical motivations of our analysis and several related works.

Major applications of the zeta-regularization approach are related to the problem of *zero point oscillations* or *Casimir effect* in Quantum Field Theory (QFT).

In his 1948 paper [7] the Dutch physicists H. B. G. Casimir pointed out that two parallel, neutral, perfectly conducting plates will show an attractive force. This phenomenon, which was later on named Casimir effect, originates from the variation of the electromagnetic *zero point energy* due to the boundaries represented by the plates.

In his setting, Casimir considered a box-shaped cavity with a plate inside, placed parallel to the walls of the cavity. Casimir showed that the plate interacts with the walls through a force (later referred to as *Casimir force*) which is inversely proportional to the cube of the distance between the plate and the walls.

The crucial observation in the paper [7] is the following. The energy of the cavity is given by $\frac{1}{2}\sum \hbar\omega$ (resp. $\frac{1}{2}\sum \hbar\omega'$) where ω (resp. ω') are the resonant frequencies of the cavity with (resp. without) the plate inserted in it, and the sum runs over all the possible frequencies. Even though the sums $\frac{1}{2}\sum \hbar\omega$ and $\frac{1}{2}\sum \hbar\omega'$ diverge, a finite value (which depends on the position of the plate) can be assigned to the difference of these energies. The Casimir force was indeed computed by taking the derivative of this finite energy difference with respect to the parameter associated to the position of the plate.

Nowadays the term Casimir effect refers to a wide class of phenomena that are associated to the variation of the zero point energy or zero point oscillations in QFT, where a quantized field can be described as a set of oscillators. In a bounded region of the space, for example, the zero point energy of the field is given by a sum of the form $\sum_j \omega_j$, where ω_j are all the possible frequencies of the oscillators and the sum runs over an infinite set of quantum numbers (here denoted by j). This series is, in general, divergent. Casimir's approach allows to regularize, by subtraction, this divergent quantity and extract the relevant information from the regularized energy.

The applications of Casimir's regularization are extremely numerous and the literature on the subject is massive. We refer to the monographs [4, 6, 25] for an exhaustive discussion on this topic and a list of related references. Here we just point out the evident relation between the divergent series in the Casimir effect and zeta-regularization techniques. Indeed, Casimir's force can be computed by regularizing a series of the form given in Eq. (2) through analytic continuation, and then taking the limit $\lim_{s\to-1}\zeta(A;s)$ (see, e.g., [12]).

The first attempts to regularize sums involving the eigenvalues of elliptic operators through analytic continuation date back to the works of Minakshisundaram and Pleijel [27, 28]. A first example of an application of zeta-regularization to investigate geometrical properties of manifolds is in [33], where the authors used it to compute the analytic torsion of a smooth, compact manifold.

One of the first applications to QFT is in [10] to compute the effective Lagrangian and the energy-momentum tensor associated to a scalar field in a De Sitter background. In [10], the authors point out that this regularization procedure may produce a result different from the one obtained by dimensional regularization.

Indeed, shortly afterwards zeta-regularization was discussed by Hawking, see [20], as a method to resolve the ambiguity in the dimensional regularization of path integrals for fields in curved spacetime. A slightly different (and to some extent more rigorous) formulation of Hawking's approach was developed by Wald in [37].

Temperature effects in the classical Casimir effect were first investigated by Fierz [18] and Mehra [24]. The general dependence on temperature in QFT, instead, was first discussed in [11]. A more recent work in this direction is [31].

More recently, the zeta-regularization approach was presented in [13–17] as a tool to cure the divergences in the vacuum expectation value of both local and global observables in QFT.

One of the first attempts at using models with singular potentials (delta-interactions) to compute the energy momentum tensor is in [23]. The same model was taken up again in [5]. Delta type interactions intuitively model semitransparent walls. From a mathematical point of view they offer a two-fold advantage: in a certain sense they are less singular than pure Dirichlet conditions; moreover they produce highly solvable models, i.e. are simple enough to perform explicit computations. In [19] the authors compute the Casimir energy of a boson field in the presence of two semitransparent walls in spatial dimension $d = 1$ and of a delta interaction supported by a circle in dimension $d = 2$. In a similar setting, but in $d = 1$ and $d = 3$ space dimensions, the Casimir energy and the pressure for a massless scalar field are explicitly computed in [26]. See [8] for a similar analysis in the case of a delta interaction supported on a cylindrical shell. A systematic analysis of the configuration with two semitransparent walls (with a discussion of the limit in which the boundary conditions become of Dirichlet type) is in [30].

We remark that none of the works mentioned in the discussion above uses the relative-zeta function regularization scheme. The general theory of the relative-zeta approach was developed by Müller in the seminal paper [29].

When computing the relative zeta function $\zeta_1(s)$, however, we will not use directly the results in [29] but we will follow the equivalent approach presented in [36]. Our choice relies on the fact that in [29] the relative-zeta function is computed by exploiting its relation with the difference of the semigroups $e^{-tA_\alpha} - e^{-tA_0}$; in [36], instead, it is obtained by working with the difference of the resolvents

$$R_\alpha(z) - R_0(z) := (A_\alpha - z)^{-1} - (A_0 - z)^{-1}.$$

In our setting the theory of self-adjoint extensions of symmetric operators, see, e.g. [32], allows us to obtain an explicit formula for $R_\alpha(z) - R_0(z)$, see Sect. 2, and perform exact calculations in a relatively easy way.

We conclude by mentioning few works in which the relative zeta function is used in a setting with singular interactions supported by points: [1] where the case of a point potential in the half-space is discussed; and [2] where the authors analyze the combined effect of the Coulomb together with a point potential, both centered at the origin.

The paper is structured as follows. In Sect. 2 we introduce the model and obtain an explicit formula for the resolvent of the operator A_α, in terms of the resolvent of

A_0. In Sect. 3 we obtain a formula for the relative zeta function and study its analytic continuation. In Sect. 4 we give a formula for the thermal Casimir energy; moreover we compute it explicitly in the case in which the function α is the characteristic function of an interval. We conclude the paper with an Appendix in which we discuss the case $\alpha = constant$.

2 The General Framework

We work in $d \geq 2$ spatial dimensions and write $\mathbf{x} \equiv (x^i)_{i=1,\ldots,d}$ to denote points in $\mathbf{R}^d$. We identify the points of the plane π defined in Eq. (4) with $\mathbf{x}_\parallel \equiv (x^2, \ldots, x^d) \in \mathbf{R}^{d-1}$. Moreover, we shall use the notations

$$(x^1, \mathbf{x}_\parallel) \equiv \mathbf{x} \in \mathbf{R}^d \equiv \mathbf{R} \times \mathbf{R}^{d-1}. \tag{6}$$

We denote by $\mathscr{F}$ and $\mathscr{F}^{-1}$ the distributional Fourier and inverse Fourier transform defined on integrable functions as

$$\mathscr{F}\varphi(\mathbf{k}) := \int_{\mathbf{R}^d} d\mathbf{x}\, e^{-i\mathbf{k}\cdot\mathbf{x}} \varphi(\mathbf{x}) \,, \qquad \mathscr{F}^{-1}\varphi(\mathbf{x}) := \int_{\mathbf{R}^d} d\mathbf{k}\, \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^d}\, \varphi(\mathbf{k}).$$

Notice that, with the above choice, the convolution of two functions φ, ψ fulfills

$$\mathscr{F}(\varphi * \psi)(\mathbf{k}) = \mathscr{F}\varphi(\mathbf{k})\, \mathscr{F}\psi(\mathbf{k}) \,.$$

The free Laplacian on $\mathbf{R}^d$ is the self-adjoint operator

$$A_0 := -\Delta : \mathrm{Dom}(A_0) \subset L^2(\mathbf{R}^d) \to L^2(\mathbf{R}^d) \,,$$

where $\mathrm{Dom}(A_0) = H^2(\mathbf{R}^d)$ (the Sobolev space of order two); the associated resolvent is the bounded operator

$$R_0(z) := (A_0 - z)^{-1} : L^2(\mathbf{R}^d) \to H^2(\mathbf{R}^d) \,, \qquad z \in \mathbf{C} \setminus [0, +\infty) \,.$$

Throughout the paper we consider the natural determination of the argument for complex numbers, i.e. $\arg : \mathbf{C} \setminus [0, +\infty) \to (0, 2\pi)$; furthermore, for any $z \in \mathbf{C} \setminus [0, +\infty)$, we always use the notation $\sqrt{z}$ to denote the principal square root, i.e. the one with positive imaginary part.

As well known, the action of $R_0(z)$ can be expressed in terms of the corresponding convolution kernel as $R_0(z)\varphi = \mathscr{R}_0(z) * \varphi$, where $\mathscr{R}_0(z; \mathbf{x}) = \frac{1}{2\pi}\big(\frac{-i\sqrt{z}}{2\pi|\mathbf{x}|}\big)^{d/2-1} K_{d/2-1}(-i\sqrt{z}\,|\mathbf{x}|)$ (K_ν is the modified Bessel function of second kind of order ν). We also recall that the Fourier transform of $\mathscr{R}_0(z; \cdot)$ is given by $(\mathscr{F}\mathscr{R}_0(z))(\mathbf{k}) = (|\mathbf{k}|^2 - z)^{-1}$.

Together with the notation introduced in (6), we shall often write

$$(k_1, \mathbf{k}_\parallel) \equiv \mathbf{k} \,\in\, \mathbf{R}^d \equiv \mathbf{R} \times \mathbf{R}^{d-1} \;.$$

Next, let us consider a non-negative, piecewise continuous, and compactly supported function α such that, for some $\delta > 0$, it holds true:

$$\alpha(\rho) > \delta \quad \forall \rho \in \mathrm{supp}(\alpha). \tag{7}$$

The trace on the hyperplane $\pi = \{\mathbf{x} \in \mathbf{R}^d \,|\, x^1 = 0\}$ is the unique linear bounded operator

$$\tau_\pi : H^r(\mathbf{R}^d) \to H^{r-\frac{1}{2}}(\mathbf{R}^{d-1})\,, \qquad r > 1/2\,,$$

such that, for any continuous φ there holds

$$(\tau_\pi \varphi)(\mathbf{x}_\parallel) = \varphi(0, \mathbf{x}_\parallel)\;, \qquad \mathbf{x}_\parallel \in \mathbf{R}^{d-1}\;.$$

Here and below $H^s(\Omega)$, $s \in \mathbf{R}$, denotes the usual scale of Sobolev-Hilbert spaces on the open subset $\Omega \subseteq \mathbf{R}^n$. In particular, considering the Sobolev spaces on the half spaces $\mathbf{R}^d_\pm := \{\mathbf{x} \in \mathbf{R}^d \,|\, \pm x^1 > 0\}$, one introduces the lateral traces

$$\tau_\pi^\pm : H^r(\mathbf{R}^d_\pm) \to H^{r-\frac{1}{2}}(\mathbf{R}^{d-1})\,, \qquad r > 1/2\,,$$

defined as the unique linear bounded operators such that, for any continuous (up to the boundary) function on $\mathbf{R}^d_\pm$ there holds

$$(\tau_\pi^\pm \varphi)(\mathbf{x}_\parallel) = \varphi(0^\pm, \mathbf{x}_\parallel)\;, \qquad \mathbf{x}_\parallel \in \mathbf{R}^{d-1}\;.$$

Setting

$$H^r(\mathbf{R}^d \backslash \pi) := H^r(\mathbf{R}^d_-) \oplus H^r(\mathbf{R}^d_+)\,,$$

one has that $\varphi = \varphi_- \oplus \varphi_+ \in H^r(\mathbf{R}^d \backslash \pi)$, $1/2 < r < 3/2$, belongs to $H^r(\mathbf{R}^d)$ if and only if $\tau_\pi^- \varphi_- = \tau_\pi^+ \varphi_+$; in this case $\tau_\pi^\pm \varphi_\pm = \tau_\pi \varphi$.

To proceed, consider the free Laplacian on $\mathbf{R}^{d-1}$, indicated hereafter with $-\Delta_\parallel$; since its spectrum coincides with the half-line $[0, +\infty)$, one can define via standard functional calculus the bounded self-adjoint operator

$$\alpha(-\Delta_\parallel) : L^2(\mathbf{R}^{d-1}) \to L^2(\mathbf{R}^{d-1})\,.$$

We use such an operator to define a self-adjoint singular perturbation of the free Laplacian $A_\alpha : \mathrm{Dom}(A_\alpha) \subset L^2(\mathbf{R}^d) \to L^2(\mathbf{R}^d)$ with domain

$$\begin{aligned}\mathrm{Dom}(A_\alpha) =\{\varphi = \varphi_- \oplus \varphi_+ \in H^2(\mathbf{R}^d\backslash\pi) \mid \tau_\pi^-\varphi_- = \tau_\pi^+\varphi_+ \\ \tau_\pi^+\partial_1\varphi_+ - \tau_\pi^-\partial_1\varphi_- = \alpha(-\Delta_\|)\tau_\pi\varphi\}\,.\end{aligned} \tag{8}$$

Similar models, with momentum dependent delta-interactions supported on spherical shells, were studied in [3, 9, 35].

Let us consider, for any $z \in \mathbf{C}\backslash[0,+\infty)$, the bounded operator

$$\breve{G}_z : L^2(\mathbf{R}^d) \to H^{3/2}(\mathbf{R}^{d-1})\,, \qquad \breve{G}_z\varphi := \tau_\pi R_0(z)\varphi.$$

Next, consider the adjoint of $\breve{G}_{\bar z}$ with respect to the $H^{-3/2}(\mathbf{R}^{d-1})$-$H^{3/2}(\mathbf{R}^{d-1})$ duality $(\cdot|\cdot)$, that is the unique bounded operator

$$G_z : H^{-3/2}(\mathbf{R}^{d-1}) \to L^2(\mathbf{R}^d)\,,$$

fulfilling

$$\langle G_z q|\varphi\rangle_{L^2(\mathbf{R}^d)} = (q|\breve{G}_{\bar z}\varphi) \qquad q \in H^{-3/2}(\mathbf{R}^{d-1}), \varphi \in L^2(\mathbf{R}^d).$$

One can easily check that G_z corresponds to the single layer operator of the hyperplane π.

Let us now introduce a convenient representation of $R_0(z)$; since it is a bounded operator, it suffices to consider its action on any $\varphi = \varphi_1 \otimes \varphi_\|$ belonging to the dense subset $\mathscr{S}(\mathbf{R}) \otimes \mathscr{S}(\mathbf{R}^{d-1})$. Recalling the explicit representation of the kernel of the resolvent of the free 1-dimensional Laplacian Δ_1, one has

$$\begin{aligned}&(R_0(z)\varphi_1 \otimes \varphi_\|)\,(x^1,\mathbf{x}_\|) = ((A_0 - z)^{-1}\varphi_1 \otimes \varphi_\|)\,(x^1,\mathbf{x}_\|) \\ =&\frac{1}{(2\pi)^d}\int_{\mathbf{R}^{d-1}} d\mathbf{k}_\|\; e^{i\,\mathbf{k}_\|\cdot\mathbf{y}_\|}\mathscr{F}\varphi_\|(\mathbf{k}_\|)\left(\int_{\mathbf{R}} dk_1\;\frac{e^{ik_1x^1}\,\mathscr{F}\varphi_1(k_1)}{k_1^2 + |\mathbf{k}_\||^2 - z}\right) \\ =&\frac{1}{(2\pi)^{d-1}}\int_{\mathbf{R}^{d-1}} d\mathbf{k}_\|\; e^{i\,\mathbf{k}_\|\cdot\mathbf{y}_\|}\mathscr{F}\varphi_\|(\mathbf{k}_\|)\left(\left(-\Delta_1 + |\mathbf{k}_\||^2 - z\right)^{-1}\varphi_1\right)(x^1) \\ =&\frac{1}{(2\pi)^{d-1}}\int_{\mathbf{R}^{d-1}} d\mathbf{k}_\|\; e^{i\,\mathbf{k}_\|\cdot\mathbf{y}_\|}\mathscr{F}\varphi_\|(\mathbf{k}_\|)\left(\int_{\mathbf{R}} dy^1\;\frac{ie^{i\sqrt{z-|\mathbf{k}_\||^2}\;|x^1-y^1|}}{2\sqrt{z-|\mathbf{k}_\||^2}}\;\varphi_1(y^1)\right) \\ =&\frac{i}{2}\left(\left(\int_{\mathbf{R}} dy^1\;\varphi_1(y^1)\,e^{i|x^1-y^1|\,(z+\Delta_\|)^{1/2}}\right)\,(z+\Delta_\|)^{-1/2}\varphi_\|\right)(\mathbf{x}_\|)\,.\end{aligned}$$

This gives

$$(\breve{G}_z\varphi_1 \otimes \varphi_\|)(\mathbf{x}_\|) = \frac{i}{2}\left(\left(\int_{\mathbf{R}} dy^1\ \varphi_1(y^1)\, e^{i|y^1|\,(z+\Delta_\|)^{1/2}}\right)(z+\Delta_\|)^{-1/2}\varphi_\|\right)(\mathbf{x}_\|)$$

and so

$$(G_z q)(x^1, \mathbf{x}_\|) = \frac{i}{2}\left(e^{i|x^1|\,(z+\Delta_\|)^{1/2}}(z+\Delta_\|)^{-1/2}q\right)(\mathbf{x}_\|)\,. \tag{9}$$

We note that the corresponding integral kernels are of convolution type in the variables $\mathbf{x}_\|$ and $\mathbf{y}_\|$, i.e.

$$(\breve{G}_z\varphi)(\mathbf{x}_\|) = \int_{\mathbf{R}} dy^1 \int_{\mathbf{R}^{d-1}} d\mathbf{y}_\|\ \mathscr{G}_z(y^1, \mathbf{x}_\| - \mathbf{y}_\|)\varphi(y^1, \mathbf{y}_\|) = \int_{\mathbf{R}} dy^1 (\mathscr{G}_z(y^1,\cdot) * \varphi(y^1,\cdot))(\mathbf{x}_\|)\,,$$

$$(G_z q)(x^1, \mathbf{x}_\|) = \int_{\mathbf{R}^{d-1}} d\mathbf{y}_\|\ \mathscr{G}_z(x^1, \mathbf{x}_\| - \mathbf{y}_\|)q(\mathbf{y}_\|) = (\mathscr{G}_z(x^1,\cdot) * q)(\mathbf{x}_\|)\,.$$

Moreover the Fourier transform (on $\mathbf{x}_\|$) of the function $\mathscr{G}_z(x^1, \mathbf{x}_\|)$ is given by

$$(\mathscr{F}\mathscr{G}_z(x^1,\cdot))(\mathbf{k}_\|) = \frac{i e^{i|x^1|\sqrt{z-|\mathbf{k}_\||^2}}}{2\sqrt{z-|\mathbf{k}_\||^2}}.$$

By Eq. (9), one infers that $\tau_\pi G_z$, $z \in \mathbf{C}\setminus[0,+\infty)$, extends to a well defined pseudodifferential operator M_z of order (-1) defined on the whole scale of Sobolev-Hilbert spaces on $\mathbf{R}^{d-1}$:

$$M_z : H^r(\mathbf{R}^{d-1}) \to H^{r+1}(\mathbf{R}^{d-1})\,,\quad M_z := \frac{i}{2}\,(z+\Delta_\|)^{-1/2}\,.$$

Then, by using M_z, we define, for any $z \in \mathbf{C}\setminus[0,+\infty)$,

$$W_\alpha(z) := -\alpha(-\Delta_\|)\Big(1+\alpha(-\Delta_\|)M_z\Big)^{-1}\ :\ L^2(\mathbf{R}^{d-1})\ \to\ L^2(\mathbf{R}^{d-1})\,.$$

Notice that $W_\alpha(z)$ is a bounded operator since, by functional calculus, $W_\alpha(z) = w_z(-\Delta_\|)$, where

$$w_z(\rho) = -\frac{\alpha(\rho)\sqrt{z-\rho}}{\sqrt{z-\rho}+i\alpha(\rho)/2}$$

and $w_z \in L^\infty(0,+\infty)$ for any $z \in \mathbf{C}\setminus[0,+\infty)$. Indeed, the associated convolution kernel is given by $\mathscr{W}_\alpha(z;\mathbf{x}_\| - \mathbf{y}_\|)$, with $(\mathscr{F}\mathscr{W}_\alpha(z;\cdot))(\mathbf{k}_\|) = w_z(|\mathbf{k}_\||^2)$.

Finally, for any $z \in \mathbf{C} \setminus [0, +\infty)$ we define the bounded linear operator $R_\alpha(z)$ by

$$R_\alpha(z) : L^2(\mathbf{R}^d) \to L^2(\mathbf{R}^d)\,, \quad R_\alpha(z) = R_0(z) + \, G_z\, W_\alpha(z)\, \breve{G}_z\,.$$

By the results provided in [32, Sect. 2], applied to the case in which the map there denoted by τ is given by $\tau := \sqrt{\alpha}(-\Delta_\parallel)\tau_\pi$, one gets that R_α is a pseudo-resolvent, i.e. it satisfies the resolvent identity $R_\alpha(w) - R_\alpha(z) = (z-w)R_\alpha(w)R_\alpha(z)$. Moreover, by Eq. (9),

$$\tau_\pi^- \partial_1 G_z q - \tau_\pi^+ \partial_1 G_z q = q \tag{10}$$

and so $\mathrm{Ran}(G_z) \cap H^2(\mathbf{R}^d) = \{0\}$, i.e. $R_\alpha(z)$ is injective. In conclusion, since $R_\alpha(\bar{z}) = R_\alpha(z)^*$, $R_\alpha(z)$ is the resolvent of the (z-independent) self-adjoint operator $A_\alpha := R_\alpha(z)^{-1} + z$ defined on the domain $\mathrm{Dom}(A_\alpha) := \mathrm{Ran}(R_\alpha(z))$. Setting $G := G_{-1}$ and $W_\alpha := W_\alpha(-1)$, one has

$$\mathrm{Dom}(A_\alpha) = \{\varphi \in L^2(\mathbf{R}^d) \mid \varphi = \varphi_0 + G W_\alpha \tau_\pi \varphi_0\,,\ \varphi_0 \in H^2(\mathbf{R}^d)\} \tag{11}$$

and, by the identity $R_\alpha(-1)(A_0 + 1)\varphi_0 = \varphi_0 + G W_\alpha \tau_\pi \varphi_0$,

$$(A_\alpha + 1)\varphi = (A_0 + 1)\varphi_0\,. \tag{12}$$

The representation of $\mathrm{Dom}(A_\alpha)$ given in (11) coincides with (8) by $\tau_\pi^- G q = \tau_\pi^+ G q$ (which is consequence of Eq. (9)) and by the identities (here we use Eq. (10) and the definition of W_α)

$$\begin{aligned}
&\tau_\pi^+ \partial_1 \varphi - \tau_\pi^- \partial_1 \varphi = \tau_\pi^+ \partial_1 G W_\alpha \tau_\pi \varphi_0 - \tau_\pi^- \partial_1 G W_\alpha \tau_\pi \varphi_0 = -W_\alpha \tau_\pi \varphi_0 \\
=& -(1 + \alpha(-\Delta_\parallel)\tau_\pi G) W_\alpha \tau_\pi \varphi_0 + \alpha(-\Delta_\parallel)\tau_\pi G W_\alpha \tau_\pi \varphi_0 \\
=& \alpha(-\Delta_\parallel)\tau_\pi \varphi_0 + \alpha(-\Delta_\parallel)\tau_\pi G W_\alpha \tau_\pi \varphi_0 = \alpha(-\Delta_\parallel)\tau_\pi \varphi\,.
\end{aligned}$$

Moreover, since $(-\Delta + 1)G = \delta_\pi$, where δ_π denotes the tempered distribution defined by $\delta_\pi(\phi) := \int_{\mathbf{R}^{d-1}} \phi(0, \mathbf{x}_\parallel)\, d\mathbf{x}_\parallel$, $\phi \in \mathscr{S}(\mathbf{R}^d)$, by Eq. (12) one has

$$A_\alpha \varphi = A_0 \varphi_0 + G W_\alpha \tau_\pi \varphi_0 = -\Delta\varphi - W_\alpha \tau_\pi \varphi_0 \delta_\pi = -\Delta\varphi + \alpha(-\Delta_\parallel)\tau_\pi \varphi \delta_\pi\,.$$

3 The Relative Zeta Function

In this section we obtain an explicit expression for the relative zeta function $\zeta_1(s)$. The formula is given in Eq. (16) and expresses the relative zeta function as an integral of the relative spectral measure $e_1(v)$. This identity holds true for the values of s in the strip (17). The function $e_1(v)$ is defined in Eq. (15) and computed explicitly in Sect. 3.1. In the same section we also obtain the asymptotic expansions of the function $e_1(v)$ for $v \to 0^+$ and $v \to +\infty$. We will use these asymptotic expansions in Sect. 3.3 to obtain the analytic continuation of the function $\zeta_1(s)$ to the strip defined by Eq. (42).

Denote by $R^{rel}(z)$ the operator

$$R^{rel}(z) := R_\alpha(z) - R_0(z) \qquad z \in \mathbf{C} \setminus [0, +\infty).$$

The integral kernel of $R^{rel}(z)$ is of convolution type on the variables $\mathbf{x}_\parallel$ and $\mathbf{y}_\parallel$ and it is given by

$$\mathscr{R}^{rel}(z; x^1, y^1, \mathbf{x}_\parallel - \mathbf{y}_\parallel) = (\mathscr{G}_z(x^1, \cdot) * \mathscr{W}_\alpha(z; \cdot) * \mathscr{G}_z(y^1, \cdot))(\mathbf{x}_\parallel - \mathbf{y}_\parallel)$$
$$= \frac{1}{4(2\pi)^{d-1}} \int_{\mathbf{R}^{d-1}} d\mathbf{k}_\parallel \; e^{i\mathbf{k}_\parallel \cdot (\mathbf{x}_\parallel - \mathbf{y}_\parallel)} \frac{\alpha(|\mathbf{k}_\parallel|^2)\, e^{i(|x^1|+|y^1|)\sqrt{z-|\mathbf{k}_\parallel|^2}}}{\sqrt{z-|\mathbf{k}_\parallel|^2}\left(\sqrt{z-|\mathbf{k}_\parallel|^2} + i\alpha(|\mathbf{k}_\parallel|^2)/2\right)} \,. \tag{13}$$

To compute the relative zeta function defined in Eq. (5) we will compute first the function

$$r_1(z) := \int_{\mathbf{R}} dx^1 \; \mathscr{R}^{rel}(z; x^1, x^1, \mathbf{0}) \qquad z \in \mathbf{C} \setminus [0, +\infty). \tag{14}$$

Then we will show that the *relative spectral measure*[1]

$$e_1(v) := \frac{v}{i\pi} \lim_{\varepsilon \to 0^+} \Big[r_1(v^2 + i\varepsilon) - r_1(v^2 - i\varepsilon) \Big] \tag{15}$$

is well defined for any $v > 0$, see Sect. 3.1. Finally, is Sect. 3.2, we shall prove that the function $\zeta_1(s)$ can be expressed through the following fundamental formula

$$\zeta_1(s) = \int_0^{+\infty} dv \; v^{-2s} \, e_1(v) \tag{16}$$

for any complex s in the strip

$$\left\{ s \in \mathbf{C} \;\middle|\; -\frac{1}{2} < \operatorname{Re} s < \frac{d-1}{2} \right\} . \tag{17}$$

Formula (16), together with the asymptotic expansions of $e_1(v)$ for $v \to 0^+$ and $v \to +\infty$, see Eqs. (30) and (31), can be used to obtain the analytic continuation of the map $s \to \zeta_1(s)$ outside the strip (17), see Eqs. (41)–(43).

---

[1]We remark that here we are slightly abusing terminology, as "relative spectral measure" usually denotes the function $e(v) := \frac{v}{i\pi} \lim_{\varepsilon \to 0^+} \operatorname{Tr}\,(R(v^2 + i\varepsilon) - R_0(v^2 - i\varepsilon))$.

We start by computing function $r_1(z)$ defined in Eq. (14).

For notational convenience, we introduce the rescaled function

$$\tilde{\alpha}(\rho) := \frac{1}{2}\,\alpha(\rho) \qquad (\rho \in [0, +\infty))\ . \tag{18}$$

Setting $y^1 = x^1$ and $\mathbf{y}_\parallel = \mathbf{x}_\parallel$ in Eq. (13) and integrating over x^1, we are left with

$$r_1(z) = \frac{i\pi}{(2\pi)^d}\int_{\mathbf{R}^{d-1}} d\mathbf{k}_\parallel\, \frac{\tilde{\alpha}(|\mathbf{k}_\parallel|^2)}{(z-|\mathbf{k}_\parallel|^2)\left(\sqrt{z-|\mathbf{k}_\parallel|^2}+i\tilde{\alpha}(|\mathbf{k}_\parallel|^2)\right)}\ . \tag{19}$$

Note that for any $z \in \mathbf{C} \setminus [0, +\infty)$, we have $\mathrm{Im}\,\sqrt{z-|\mathbf{k}_\parallel|^2} > 0$ and recall that the function $\alpha(\rho)$ is compactly supported by assumption. Hence, one can exchange order of integration and perform the integral over x^1.

Next, passing to polar coordinates and considering the change of variable $\rho := |\mathbf{k}_\parallel|^2 \in (0, +\infty)$, one obtains

$$r_1(z) = \frac{i\pi^2}{(2\pi)^{\frac{d+3}{2}}\,\Gamma(\frac{d-1}{2})}\int_0^{+\infty} d\rho\, \frac{\rho^{\frac{d-3}{2}}\,\tilde{\alpha}(\rho)}{(z-\rho)(\sqrt{z-\rho}+i\tilde{\alpha}(\rho))}\ , \tag{20}$$

where $\Gamma(\cdot)$ denotes the Euler Gamma function.

3.1 *The Relative Spectral Measure and Its Asymptotic Expansion*

In this section we obtain an explicit formula for the function $e_1(v)$ defined in Eq. (15) (see Eq. (26) below). Then compute its asymptotic expansion for $v \to 0^+$, see Eq. (30), and for $v \to +\infty$, see Eq. (31).

First of all, let us point out the trivial identity

$$\frac{\tilde{\alpha}(\rho)}{(z-\rho)(\sqrt{z-\rho}+i\tilde{\alpha}(\rho))} = -\frac{i}{z-\rho} + \frac{i}{\sqrt{z-\rho}(\sqrt{z-\rho}+i\tilde{\alpha}(\rho))}.$$

In view of the above identity, and recalling Eq. (20), the difference $r_1(v^2+i\varepsilon) - r_1(v^2-i\varepsilon)$ can be expressed via simple algebraic manipulations as

$$r_1(v^2+i\varepsilon) - r_1(v^2-i\varepsilon) = \frac{i\pi^2}{(2\pi)^{\frac{d+3}{2}}\,\Gamma\left(\frac{d-1}{2}\right)}\big(E_1(\varepsilon; v) + E_2(\varepsilon, v) + E_3(\varepsilon; v)\big)$$

where

$$E_1(\varepsilon; v) := -\int_{\text{supp}\alpha} d\rho \rho^{\frac{d-3}{2}} \frac{2\varepsilon}{(v^2-\rho)^2+\varepsilon^2} \, ,$$

$$E_2(\varepsilon; v) := i \int_{\text{supp}\alpha} d\rho \frac{\rho^{\frac{d-3}{2}}}{\sqrt{v^2-\rho+i\varepsilon}+i\tilde{\alpha}(\rho)} \left(\frac{1}{\sqrt{v^2-\rho+i\varepsilon}} - \frac{1}{\sqrt{v^2-\rho-i\varepsilon}} \right) ,$$

$$E_3(\varepsilon; v) := i \int_{\text{supp}\alpha} d\rho \frac{\rho^{\frac{d-3}{2}}}{\sqrt{v^2-\rho-i\varepsilon}} \times \left(\frac{1}{\sqrt{v^2-\rho+i\varepsilon}+i\tilde{\alpha}(\rho)} - \frac{1}{\sqrt{v^2-\rho-i\varepsilon}+i\tilde{\alpha}(\rho)} \right) .$$

We study the convergence for $\varepsilon \to 0^+$ term by term.

For the term $E_1(\varepsilon; v)$ we use the fact that $\frac{2\varepsilon}{(v^2-\rho)^2+\varepsilon^2} \to \pi\delta(\rho - v^2)$ and the fact that, $\rho^{\frac{d-3}{2}} \chi_{\text{supp}\alpha}(\rho)$ is piecewise continuous (here and below $\chi_{\text{supp}\alpha}(\cdot)$ denotes the characteristic function of suppα) to get (see, e.g., [21, Ex. 1.13])

$$\lim_{\varepsilon\to 0^+} E_1(\varepsilon; v) = -2\pi v^{d-3} \chi_{\text{supp}\alpha}(v^2) \tag{21}$$

To compute the limit of $E_2(\varepsilon; v)$ and $E_3(\varepsilon; v)$ requires a bit more work. We start by recalling the following inequalities, holding for some $C > 0$:

$$|\sqrt{\lambda+i\varepsilon} - \sqrt{\lambda-i\varepsilon} - 2\sqrt{\lambda}| \le C\sqrt{\varepsilon} \qquad \forall\lambda > 0 \, ; \tag{22}$$

$$|\sqrt{\lambda+i\varepsilon} - \sqrt{\lambda-i\varepsilon}| \le C\sqrt{\varepsilon} \qquad \forall\lambda < 0 \, . \tag{23}$$

Next, we analyze the term $E_2(\varepsilon; v)$. We note the identity

$$\begin{aligned} &E_2(\varepsilon; v) - i \int_{\text{supp}\alpha\cap(0,v^2)} d\rho \frac{\rho^{\frac{d-3}{2}}}{\sqrt{v^2-\rho+i\varepsilon}+i\tilde{\alpha}(\rho)} \frac{2\sqrt{v^2-\rho}}{\sqrt{(v^2-\rho)^2+\varepsilon^2}} \\ &= i \int_{\text{supp}\alpha\cap(0,v^2)} d\rho \frac{\rho^{\frac{d-3}{2}}}{\sqrt{v^2-\rho+i\varepsilon}+i\tilde{\alpha}(\rho)} \frac{\sqrt{v^2-\rho+i\varepsilon} - \sqrt{v^2-\rho-i\varepsilon} - 2\sqrt{v^2-\rho}}{\sqrt{(v^2-\rho)^2+\varepsilon^2}} \\ &+ i \int_{\text{supp}\alpha\cap(v^2,+\infty)} d\rho \frac{\rho^{\frac{d-3}{2}}}{\sqrt{v^2-\rho+i\varepsilon}+i\tilde{\alpha}(\rho)} \frac{\sqrt{v^2-\rho+i\varepsilon} - \sqrt{v^2-\rho-i\varepsilon}}{\sqrt{(v^2-\rho)^2+\varepsilon^2}} , \end{aligned}$$

where we used the fact that, due to our definition of the square root, we have that $\sqrt{v^2-\rho+i\varepsilon}\sqrt{v^2-\rho-i\varepsilon} = -\sqrt{(v^2-\rho^2)+\varepsilon^2}$. To proceed, let us recall that the square root is taken with positive imaginary part and that $\alpha(\rho) > \delta$ for all

$\rho \in \mathrm{supp}\alpha$, see Eq. (7); then, by using the inequalities (22)–(23), we infer

$$\left| E_2(\varepsilon; v) - i \int_{\mathrm{supp}\alpha\cap(0,v^2)} d\rho \frac{\rho^{\frac{d-3}{2}}}{\sqrt{v^2-\rho+i\varepsilon}+i\tilde{\alpha}(\rho)} \frac{2\sqrt{v^2-\rho}}{\sqrt{(v^2-\rho)^2+\varepsilon^2}} \right|$$
$$\leq \frac{C}{\delta}\left(\int_{\mathrm{supp}\alpha} d\rho \rho^{\frac{d-3}{2}} \frac{\sqrt{\varepsilon}}{\sqrt{(v^2-\rho)^2+\varepsilon^2}} \right) \leq \frac{C\varepsilon^{1/4}}{\delta} \int_{\mathrm{supp}\alpha} d\rho \rho^{\frac{d-3}{2}} \frac{1}{|v^2-\rho|^{3/4}}$$
$$\leq C(\alpha, d)\varepsilon^{1/4} .$$

Since, by dominated convergence, one has

$$\lim_{\varepsilon\to 0^+} i \int_{\mathrm{supp}\alpha\cap(0,v^2)} d\rho \frac{\rho^{\frac{d-3}{2}}}{\sqrt{v^2-\rho+i\varepsilon}+i\tilde{\alpha}(\rho)} \frac{2\sqrt{v^2-\rho}}{\sqrt{(v^2-\rho)^2+\varepsilon^2}}$$
$$= i \int_{\mathrm{supp}\alpha\cap(0,v^2)} d\rho \frac{\rho^{\frac{d-3}{2}}}{\sqrt{v^2-\rho}+i\tilde{\alpha}(\rho)} \frac{2}{\sqrt{v^2-\rho}} ,$$

we conclude that

$$\lim_{\varepsilon\to 0^+} E_2(\varepsilon, v) = i \int_{\mathrm{supp}\alpha\cap(0,v^2)} d\rho \frac{\rho^{\frac{d-3}{2}}}{\sqrt{v^2-\rho}+i\tilde{\alpha}(\rho)} \frac{2}{\sqrt{v^2-\rho}} . \tag{24}$$

Reasoning in a similar way, let us consider the identity

$$E_3(\varepsilon; v) - i \int_{\mathrm{supp}\alpha\cap(0,v^2)} d\rho \frac{\rho^{\frac{d-3}{2}}(v^2-\rho-i\varepsilon)^{-1/2} 2\sqrt{v^2-\rho}}{\left(\mathrm{Re}\,\sqrt{v^2-\rho+i\varepsilon}\right)^2 + \left(\mathrm{Im}\,\sqrt{v^2-\rho+i\varepsilon}+\tilde{\alpha}(\rho)\right)^2}$$
$$= i \int_{\mathrm{supp}\alpha\cap(0,v^2)} d\rho \frac{\rho^{\frac{d-3}{2}}(v^2-\rho-i\varepsilon)^{-1/2}(\sqrt{v^2-\rho+i\varepsilon}-\sqrt{v^2-\rho-i\varepsilon}-2\sqrt{v^2-\rho})}{\left(\mathrm{Re}\,\sqrt{v^2-\rho+i\varepsilon}\right)^2 + \left(\mathrm{Im}\,\sqrt{v^2-\rho+i\varepsilon}+\tilde{\alpha}(\rho)\right)^2}$$
$$+ i \int_{\mathrm{supp}\alpha\cap(v^2,+\infty)} d\rho \frac{\rho^{\frac{d-3}{2}}(v^2-\rho-i\varepsilon)^{-1/2}(\sqrt{v^2-\rho+i\varepsilon}-\sqrt{v^2-\rho-i\varepsilon})}{\left(\mathrm{Re}\,\sqrt{v^2-\rho+i\varepsilon}\right)^2 + \left(\mathrm{Im}\,\sqrt{v^2-\rho+i\varepsilon}+\tilde{\alpha}(\rho)\right)^2} ,$$

where we used the fact that $\mathrm{Re}\,\sqrt{v^2-\rho-i\varepsilon} = -\mathrm{Re}\,\sqrt{v^2-\rho+i\varepsilon}$ and $\mathrm{Im}\,\sqrt{v^2-\rho-i\varepsilon} = \mathrm{Im}\,\sqrt{v^2-\rho+i\varepsilon}$. This allows us to infer

$$\left| E_3(\varepsilon; v) - i \int_{\mathrm{supp}\alpha\cap(0,v^2)} d\rho \frac{\rho^{\frac{d-3}{2}}(v^2-\rho-i\varepsilon)^{-1/2} 2\sqrt{v^2-\rho}}{\left(\mathrm{Re}\,\sqrt{v^2-\rho+i\varepsilon}\right)^2 + \left(\mathrm{Im}\,\sqrt{v^2-\rho+i\varepsilon}+\tilde{\alpha}(\rho)\right)^2} \right|$$
$$\leq \frac{\sqrt{\varepsilon}}{\delta^2} \int_{\mathrm{supp}\alpha} d\rho \frac{\rho^{\frac{d-3}{2}}}{|\sqrt{v^2-\rho-i\varepsilon}|} \leq \frac{\sqrt{\varepsilon}}{\delta^2} \int_{\mathrm{supp}\alpha} d\rho \frac{\rho^{\frac{d-3}{2}}}{\sqrt{|v^2-\rho|}} \leq C(\alpha, d)\sqrt{\varepsilon}.$$

As before, by using the dominated convergence theorem, one can prove that

$$\lim_{\varepsilon\to 0^+} E_3(\varepsilon; v) = -i\int_{\mathrm{supp}\alpha\cap(0,v^2)} d\rho \frac{\rho^{\frac{d-3}{2}}}{\sqrt{v^2-\rho}}\frac{2\sqrt{v^2-\rho}}{v^2-\rho+\tilde{\alpha}(\rho)^2}. \tag{25}$$

Summing up the limits (24) and (25), we conclude

$$\lim_{\varepsilon\to 0^+} \big(E_2(\varepsilon; v) + E_3(\varepsilon; v)\big) = \int_0^{v^2} d\rho \frac{\rho^{\frac{d-3}{2}}}{\sqrt{v^2-\rho}}\frac{2\tilde{\alpha}(\rho)}{v^2-\rho+\tilde{\alpha}(\rho)^2}.$$

Taking into account also the limit (21) we get the following expression:

$$e_1(v) = \frac{\pi\ v}{(2\pi)^{\frac{d+1}{2}}\Gamma(\frac{d-1}{2})}\Big[-v^{d-3}\,\chi_{\mathrm{supp}\alpha}(v^2) + I_\alpha(v^2)\,\chi_{(0,+\infty)}(v)\Big], \tag{26}$$

where we introduced the notation

$$I_\alpha(\lambda) := \frac{1}{\pi}\int_0^\lambda d\rho\ \frac{\rho^{\frac{d-3}{2}}\,\tilde{\alpha}(\rho)}{\sqrt{\lambda-\rho}\,(\lambda-\rho+\tilde{\alpha}(\rho)^2)} \qquad \text{for any } \lambda\in(0,+\infty)\,. \tag{27}$$

Before proceeding, let us stress that due to the assumptions on α, the integral I_α can be easily checked to be finite and positive for any $\lambda \in (0, +\infty)$. In fact, by Lebesgue's dominated convergence theorem, one can infer that the map $\lambda \mapsto I_\alpha(\lambda)$ is continuous on $[0, +\infty)$.

Next, let us pass to discuss the asymptotic behavior of the map $\lambda \mapsto I_\alpha(\lambda)$ for $\lambda \to 0^+$ and $\lambda \to +\infty$. For $\lambda \to 0^+$, we have that

$$I_\alpha(\lambda) \le \frac{\|\alpha\|_\infty}{\pi\delta^2}\int_0^\lambda d\rho\ \frac{\rho^{\frac{d-3}{2}}}{\sqrt{\lambda-\rho}} \le \frac{\|\alpha\|_\infty\lambda^{\frac{d-3}{2}}}{\pi\delta^2}\int_0^\lambda d\rho\ \frac{1}{\sqrt{\lambda-\rho}} \le C(\alpha)\lambda^{\frac{d-2}{2}}.$$

Hence,

$$I_\alpha(\lambda) = O(\lambda^{\frac{d-2}{2}}) \qquad \text{for } \lambda\to 0^+\,.$$

Next we discuss the asymptotic behavior of $I_\alpha(\lambda)$ in the limit $\lambda \to +\infty$; in particular, we shall show that that there exits a family of real coefficients $(p_n)_{n=0,1,2,\ldots}$ such that, for any $N \in \{0, 1, 2, \ldots\}$,

$$I_\alpha(\lambda) = \lambda^{-3/2}\sum_{n=0}^{N} p_n\,\lambda^{-n} + O(\lambda^{-N-\frac{5}{2}}) \quad \text{for } \lambda\to+\infty\,; \tag{28}$$

for example, the first two coefficients are

$$p_0 := \frac{1}{\pi}\int_{\text{supp}\alpha} d\rho\, \rho^{\frac{d-3}{2}}\, \tilde{\alpha}(\rho)\ ,$$
$$p_1 := \frac{1}{\pi}\int_{\text{supp}\alpha} d\rho\, \rho^{\frac{d-3}{2}}\, \tilde{\alpha}(\rho)\left(\frac{3}{2}\,\rho - \tilde{\alpha}(\rho)^2\right)\ . \tag{29}$$

Keeping in mind that α is assumed to have compact support, let us fix arbitrarily $\rho_1 \in (0, +\infty)$ such that

$$\text{supp}\alpha \subseteq [0, \rho_1]\ .$$

Next, let us consider the representation (27) of $I_\alpha(\lambda)$ and notice that, for any $\lambda > \rho_1$, it can be re-expressed as

$$I_\alpha(\lambda) := \frac{\lambda^{-3/2}}{\pi}\int_0^{\rho_1} d\rho\, \frac{\rho^{\frac{d-3}{2}}\,\tilde{\alpha}(\rho)}{\sqrt{1-\frac{\rho}{\lambda}}\left(1+\frac{\tilde{\alpha}(\rho)^2-\rho}{\lambda}\right)}\ .$$

To proceed, notice that for any $N \in \{0, 1, 2, \ldots\}$ and any fixed $\rho \in (0, \rho_1)$ there exits a family of coefficients $(g_n(\rho))_{n=0,\ldots,N}$ and a Taylor-Lagrange reminder function $T_N(\rho;\cdot) : (\rho_1, +\infty) \to \mathbf{R}$, $\lambda \mapsto T_N(\rho;\lambda)$, such that

$$\frac{\tilde{\alpha}(\rho)}{\sqrt{1-\frac{\rho}{\lambda}}\left(1+\frac{\tilde{\alpha}(\rho)^2-\rho}{\lambda}\right)} = \sum_{n=0}^{N} g_n(\rho)\,\lambda^{-n} + T_N(\rho,\lambda) \quad \text{for all } \lambda > \rho_1\ .$$

Let us mention that the coefficients $g_n(\rho)$ $(n = 0, \ldots, N)$ are all determined by integer powers of $\alpha(\rho)$; for example, one has

$$g_0(\rho) := \tilde{\alpha}(\rho)\ , \qquad g_1(\rho) := \tilde{\alpha}(\rho)\left(\frac{3}{2}\,\rho - \tilde{\alpha}(\rho)^2\right), \qquad \ldots$$

Therefore, since α is assumed to be bounded, one easily infers that all the functions $\rho \mapsto g_n(\rho)$ $(n = 0, \ldots, N)$ are also uniformly bounded on $(0, \rho_1)$.

Concerning the reminder T_N, one has

$$|T_N(\rho;\lambda)| \leq S_{N+1}(\rho)\,\lambda^{-(N+1)} \qquad \text{for all } \rho \in (0, \rho_1), \lambda \in (\rho_1 + 1, +\infty)\ ,$$

where we have introduced the positive-valued function

$$S_{N+1}(\rho) := \sup_{\lambda\in(\rho_1+1,+\infty)}\left|\frac{1}{(N+1)!}\frac{d^{N+1}}{d\lambda^{N+1}}\left(\frac{\tilde{\alpha}(\rho)}{\sqrt{1-\frac{\rho}{\lambda}}\left(1+\frac{\tilde{\alpha}(\rho)^2-\rho}{\lambda}\right)}\right)\right|\ ;$$

the latter can be easily proved to be uniformly bounded on $(0, \rho_1)$.

Summing up, the above results allow to infer that

$$I_\alpha(\lambda) = \frac{\lambda^{-3/2}}{\pi} \sum_{n=0}^{N} \left(\int_0^{\lambda_0} d\rho \, \rho^{\frac{d-3}{2}} g_n(\rho) \right) \lambda^{-n} + O(\lambda^{-N-\frac{5}{2}}) \quad \text{for } \lambda \to +\infty \, ,$$

thus proving Eqs. (28)–(29).

The above results on $I_\alpha(\lambda)$, along with the explicit expression (26) of the relative spectral measure, allow to infer straightforwardly the following facts concerning the map $(0, +\infty) \to \mathbf{R}$, $v \mapsto e_1(v)$:

1. $e_1 \in C^0((0, +\infty); \mathbf{R})$; in particular, e_1 is locally bounded on $(0, +\infty)$.
2. There holds

$$e_1(v) = O(v^{d-2}) \qquad \text{for } v \to 0^+. \tag{30}$$

3. For any $N \in \{0, 1, 2, \ldots\}$, there holds the asymptotic expansion

$$e_1(v) = \frac{1}{v^2} \sum_{n=0}^{N} \tilde{p}_n \, v^{-2n} + O(v^{-2-2(N+1)}) \qquad \text{for } v \to +\infty \, , \tag{31}$$

where the real coefficients $(\tilde{p}_n)_{n=0,1,2,\ldots}$ are related to the coefficients $(p_n)_{n=0,1,2,\ldots}$ appearing in Eq. (28) by the rescaling

$$\tilde{p}_n := \frac{\pi}{(2\pi)^{\frac{d+1}{2}} \Gamma(\frac{d-1}{2})} \, p_n \, . \tag{32}$$

3.2 Relative Zeta Function in Terms of the Relative Spectral Measure

This section is devoted to the proof of identity (16).

The function $\zeta_1(s)$ is defined in terms of the integral kernel of the operator $Q^{rel} = e^{-tA_\alpha} - e^{-tA_0}$ by Eq. (5). We start by recalling the well known identity

$$\mathscr{Q}^{rel}(t; x^1, y^1, \mathbf{x}_\parallel - \mathbf{y}_\parallel) = -\frac{1}{2\pi i} \int_{\Lambda_\varepsilon} dz \, e^{-zt} \mathscr{R}^{rel}(z; x^1, y^1, \mathbf{x}_\parallel - \mathbf{y}_\parallel) \, , \tag{33}$$

where, for any $\varepsilon > 0$, Λ_ε is the contour

$$\Lambda_\varepsilon = \mathscr{C}_\varepsilon \cup \Lambda_\varepsilon^+ \cup \Lambda_\varepsilon^- \qquad \text{where}$$

$$\mathscr{C} = \{ z = \varepsilon e^{i\theta} | \ \theta \in [\pi/2, 3\pi/2] \} \, , \qquad \Lambda_\varepsilon^\pm = \{ z = \lambda \pm i\varepsilon | \ \lambda \in [0, +\infty) \},$$

and the integral over Λ_ε is taken counterclockwise. From the definition of $\zeta_1(s)$, see Eq. (5), and identity (33) one has

$$\zeta_1(s) = -\frac{1}{2\pi i\Gamma(s)} \int_0^{+\infty} dt\, t^{s-1} \int_{\mathbf{R}} dx^1 \int_{\Lambda_\varepsilon} dz\, e^{-zt} \mathscr{R}^{rel}(z; x^1, x^1, \mathbf{0}).$$

We claim that for all $\varepsilon > 0$ and $t > 0$

$$\int_{\mathbf{R}} dx^1 \int_{\Lambda_\varepsilon} dz\, e^{-zt} \mathscr{R}^{rel}(z; x^1, x^1, \mathbf{0}) = \int_{\Lambda_\varepsilon} dz\, e^{-zt} r_1(z)\ .$$

To prove the latter identity it is enough to show that the integrals can be exchanged. To this aim we note that, by Eq. (13) and our assumptions on α one has

$$\begin{aligned} &\int_{\mathbf{R}} dx^1 \int_{\Lambda_\varepsilon} dz \int_{\mathbf{R}^{d-1}} d\mathbf{k}_\parallel\ \frac{|e^{-zt}|\, \alpha(|\mathbf{k}_\parallel|^2) e^{-2|x^1|\,\mathrm{Im}\,\sqrt{z-|\mathbf{k}_\parallel|^2}}}{\left|\sqrt{z-|\mathbf{k}_\parallel|^2}\right| \left|\sqrt{z-|\mathbf{k}_\parallel|^2} + i\alpha(|\mathbf{k}_\parallel|^2)/2\right|} \\ &\qquad \le \|\alpha\|_\infty \int_{\Lambda_\varepsilon} dz \int_{\{|\mathbf{k}_\parallel|^2 \in \mathrm{supp}\alpha\}} d\mathbf{k}_\parallel\ \frac{|e^{-zt}|}{\left(\mathrm{Im}\ \sqrt{z-|\mathbf{k}_\parallel|^2}\right)^3}; \end{aligned} \tag{34}$$

moreover, using the inequality

$$\frac{1}{\mathrm{Im}\ \sqrt{z-|\mathbf{k}_\parallel|^2}} \le \frac{C}{\sqrt{\varepsilon}} \max\left\{1, \sqrt{\frac{\lambda}{\varepsilon}}, \frac{|\mathbf{k}_\parallel|}{\sqrt{\varepsilon}}\right\} \qquad \text{for all } z \in \Lambda_\varepsilon,$$

one can easily prove that the integral on the r.h.s. of Eq. (34) is bounded for all $\varepsilon > 0$ and $t > 0$. This suffices to infer that the integrals can be exchanged, as stated previously.

Next we note that, by the analyticity properties of $r_1(z)$, there exists a sequence $\varepsilon_n \to 0^+$ such that

$$\begin{aligned} \zeta_1(s) &= -\frac{1}{2\pi i\Gamma(s)} \int_0^{+\infty} dt\, t^{s-1} \int_{\Lambda_\varepsilon} dz\, e^{-zt} r_1(z) \\ &= -\frac{1}{2\pi i\Gamma(s)} \int_0^{+\infty} dt\, t^{s-1} \lim_{n\to+\infty} \int_{\Lambda_{\varepsilon_n}} dz\, e^{-zt} r_1(z). \end{aligned} \tag{35}$$

We claim that for all $t > 0$ one has

$$\frac{1}{2\pi i} \lim_{\varepsilon\to 0+} \int_{\Lambda_\varepsilon} dz\, e^{-zt} r_1(z) = -\int_0^{+\infty} dv\, e^{-v^2 t} e_1(v). \tag{36}$$

Then the identity (16) follows from Eqs. (35) and (36), by exchanging order of integration and by taking into account the identity $\frac{1}{\Gamma(s)}\int_0^\infty dt\, t^{s-1} e^{-v^2 t} = v^{-2s}$.

To prove Eq. (36) we start by noticing that for all $t > 0$

$$\int_{\Lambda_\varepsilon} dz\, e^{-zt} r_1(z) = -\lim_{\varepsilon\to 0^+}\int_0^{+\infty} d\lambda \left(e^{-(\lambda+i\varepsilon)t} r_1(\lambda+i\varepsilon) - e^{-(\lambda-i\varepsilon)t} r_1(\lambda-i\varepsilon)\right), \tag{37}$$

where we used the fact that

$$\lim_{\varepsilon\to 0^+}\int_{\mathscr{C}_\varepsilon} dz\, e^{-zt} r_1(z) = 0\,.$$

The latter claim follows from the bound

$$|r_1(\varepsilon e^{i\theta})| \le C\frac{\|\alpha\|_\infty}{\delta}\int_{\{|\mathbf{k}_\parallel|^2\in \mathrm{supp}\alpha\}} d\mathbf{k}_\parallel\, \frac{1}{\sqrt{\varepsilon^2 + |\mathbf{k}_\parallel|^4}} \qquad \forall z\in\mathscr{C}_\varepsilon,$$

where we used Eq. (19) and the fact that $|z - |\mathbf{k}_\parallel|^2|^{-1} \le (\varepsilon^2 + |\mathbf{k}_\parallel|^4)^{-1/2}$ for all $z\in\mathscr{C}_\varepsilon$. In fact, in view of the estimate $\int_{\{|\mathbf{k}_\parallel|^2\in\mathrm{supp}\alpha\}} d\mathbf{k}_\parallel\, (\varepsilon^2 + |\mathbf{k}_\parallel|^4)^{-1/2} \le C\,\varepsilon^{-3/4}$ for all $0<\varepsilon<1$ (where C is a constant that depends on d and suppα), the mentioned bound allows to infer $\left|\int_{\mathscr{C}_\varepsilon} dz\, e^{-zt} r_1(z)\right| \le C\,\varepsilon^{1/4}$, thus proving the previous claim.

To move the limit inside the integral in Eq. (37) we use dominated convergence theorem. To this aim, we use first the trivial bound

$$\begin{aligned}&\left|e^{-(\lambda+i\varepsilon)t} r_1(\lambda+i\varepsilon) - e^{-(\lambda-i\varepsilon)t} r_1(\lambda-i\varepsilon)\right| \\ &\le e^{-\lambda t}\,|2\sin(\varepsilon t) r_1(\lambda+i\varepsilon)| + e^{-\lambda t}\,|r_1(\lambda+i\varepsilon) - r_1(\lambda-i\varepsilon)|\,.\end{aligned} \tag{38}$$

Next we note that

$$e^{-\lambda t}\,|2\sin(\varepsilon t) r_1(\lambda+i\varepsilon)| \le C e^{-\lambda t} t\sqrt{\varepsilon}\frac{\|\alpha\|_\infty}{\delta}\int_{\{|\mathbf{k}_\parallel|^2\in\mathrm{supp}\alpha\}} d\mathbf{k}_\parallel \frac{1}{\left|\lambda - |\mathbf{k}_\parallel|^2\right|^{1/2}}.$$

Hence the limit for $\varepsilon\to 0^+$ of the first term at the r.h.s. of Eq. (38) is zero. On the other hand, for the second term at the r.h.s. we use, see Eq. (19),

$$\begin{aligned}|r_1(\lambda+i\varepsilon) - r_1(\lambda-i\varepsilon)| \le C\|\alpha\|_\infty\Bigg(&\frac{1}{\delta}\int_{\{|\mathbf{k}_\parallel|^2\in\mathrm{supp}\alpha\}} d\mathbf{k}_\parallel\, \frac{\varepsilon}{(\lambda - |\mathbf{k}_\parallel|^2)^2 + \varepsilon^2} \\ &+\frac{1}{\delta^2}\int_{\{|\mathbf{k}_\parallel|^2\in\mathrm{supp}\alpha\}} d\mathbf{k}_\parallel\, \frac{\left|\sqrt{\lambda - |\mathbf{k}_\parallel|^2 + i\varepsilon} - \sqrt{\lambda - |\mathbf{k}_\parallel|^2 - i\varepsilon}\right|}{\left|\lambda - |\mathbf{k}_\parallel|^2 + i\varepsilon\right|}\Bigg).\end{aligned}$$

The first term is uniformly bounded in ε. For the second term we use the inequality $\frac{\left|\sqrt{\rho+i\varepsilon}-\sqrt{\rho-i\varepsilon}\right|}{\left|\rho+i\varepsilon\right|} \leq \frac{C}{\sqrt{|\rho|}}$, which holds true for all $\rho \in \mathbf{R}$ and $\varepsilon > 0$, from which it follows that the second term is uniformly bounded as well. Identity (36) follows from the dominated convergence theorem applied to Eq. (37) together with the change of variables $\lambda \to v^2$.

3.3 Analytic Continuation of the Relative Zeta Function

In this section we obtain the analytic continuation of the relative zeta function $\zeta_1(s)$. We start with the representation (16). In view of the continuity of the map $v \mapsto e_1(v)$ on $(0, +\infty)$ and of its asymptotic behaviours for $v \to 0^+$ and $v \to +\infty$ discussed previously (see, in particular, Eqs. (30) and (31)), it appears that the integral in Eq. (16) converges for any complex s in the strip given in Eq. (17).

To proceed, let us recall the well-known fact that the asymptotic expansions of $e_1(v)$ for $v \to 0^+$ and $v \to +\infty$ can be used to construct explicitly the analytic continuation of the map $s \mapsto \zeta_1(s)$ to larger regions of the complex plane, by means of standard techniques. Let us point out that, for the applications to be discussed in the forthcoming Sect. 4, it suffices to determine the said analytic continuation of $\zeta_1(s)$ to regions with larger negative values of Re s (in particular, to a neighbour of $s = -1/2$); to this purpose, let us fix $v_0 \in (0, +\infty)$ arbitrarily and re-express the relative partial zeta function as

$$\zeta_1(s) = \zeta_1^{(<)}(s) + \zeta_1^{(>)}(s) \;,$$
$$\zeta_1^{(<)}(s) := \int_0^{v_0} dv \; v^{-2s} \; e(v) \;, \qquad \zeta_1^{(>)}(s) := \int_{v_0}^{+\infty} dv \; v^{-2s} \; e(v) \;. \tag{39}$$

Notice that the asymptotic behaviour in Eq. (30) suffices to infer that the map $s \mapsto \zeta_1^{(<)}(s)$ is analytic for Re $s < (d-1)/2$. On the other hand, the integral defining $\zeta_1^{(>)}(s)$ only converges for Re $s > -1/2$; in order to construct its analytic continuation to larger negative Re s, let us fix $N \in \{0, 1, 2, \ldots\}$ and proceed to add and subtract to the integrand in Eq. (39) the first $N + 1$ terms of the asymptotic expansion of $e_1(v)$ for $v \to +\infty$ (see Eq. (31)); we thus obtain

$$\zeta_1^{(>)}(s) = \sum_{n=0}^{N} \tilde{p}_n \int_{v_0}^{+\infty} dv \; v^{-2s-2-2n} + \int_{v_0}^{+\infty} dv \; v^{-2s} \left(e_1(v) - \frac{1}{v^2} \sum_{n=0}^{N} \tilde{p}_n \; v^{-2n} \right) .$$

Therefore, using the elementary identity

$$\int_{v_0}^{+\infty} dv \; v^{-2s-2-2n} = \frac{v_0^{-2s-2n-1}}{2s+2n+1} \quad \text{for all } s \in \mathbf{C}, n \in \mathbf{N} \text{ with Re } s > -n - \frac{1}{2} \;,$$

one obtains

$$\zeta_1^{(>)}(s) = \sum_{n=0}^{N} \frac{v_0^{-2s-2n-1}}{2s+2n+1}\,\tilde{p}_n + \int_{v_0}^{+\infty} dv\; v^{-2s}\left(e_1(v) - \frac{1}{v^2}\sum_{n=0}^{N}\tilde{p}_n\, v^{-2n}\right). \tag{40}$$

Even though the above expression was derived under the assumption Re $s > -1/2$, the following facts are apparent. On the one hand, the first term on the right-hand side of Eq. (40) is a sum of functions which are meromorphic on the whole complex plane, with only simple poles at the points $\{-1/2, -3/2, \dots, -N-1/2\}$; on the other hand, the second term in Eq. (40) is an integral which converges by construction for any Re $s > -N - 3/2$ and defines an analytic function of s in this region.

Summing up, the above arguments allow to infer that the identity

$$\zeta_1(s) = \sum_{n=0}^{N} \frac{v_0^{-2s-2n-1}}{2s+2n+1}\,\tilde{p}_n + \int_0^{v_0} dv\; v^{-2s}\, e_1(v) + \int_{v_0}^{+\infty} dv\; v^{-2s}\left(e_1(v) - \frac{1}{v^2}\sum_{n=0}^{N}\tilde{p}_n\, v^{-2n}\right) \tag{41}$$

determines the analytic continuation of the map $s \mapsto \zeta_1(s)$ to a function which is meromorphic in the larger strip

$$\left\{ s \in \mathbf{C} \;\middle|\; -\frac{3}{2} - N < \mathrm{Re}\ s < \frac{d-1}{2} \right\}\ , \tag{42}$$

with possible simple pole singularities at the points

$$\{-1/2, -3/2, \dots, -N-1/2\}\ . \tag{43}$$

4 The Thermal Casimir Energy

We work in natural units, meaning that we fix the speed of light c, the reduced Plank constant $\hbar$ and the Boltzmann constant κ as follows:

$$c := 1\ , \qquad \hbar := 1\ , \qquad \kappa := 1\ .$$

In this section we proceed to compute the renormalized Casimir energy per unit surface $\mathscr{E}(\beta)$ for a massless scalar field at temperature $T = 2\pi/\beta$ ($\beta \in (0, +\infty)$), living in $(d+1)$-dimensional spacetime. A simple adaptation of the arguments presented in [36] allows to infer that this observable is completely determined by the singular and regular parts of the Laurent expansion at $s = -1/2$ of the relative zeta function $\zeta_1(s)$, discussed in the previous section; more precisely, there holds

$$\mathscr{E}(\beta) = \frac{1}{2}\,\mathrm{Res}_0\Big|_{s=-1/2}\zeta_1(s) \; + (1 - \log(2\ell))\;\mathrm{Res}_1\Big|_{s=-1/2}\zeta_1(s) + \partial_\beta \log\eta(\beta)\;, \tag{44}$$

where $\ell \in (0, +\infty)$ is a length parameter required by dimensional arguments and

$$\log\eta(\beta) := \int_0^{+\infty} dv\;\; \log(1 - e^{-\beta v})\; e_1(v)\;. \tag{45}$$

In view of Eq. (41), here employed with $N = 0$ and any fixed $v_0 \in (0, +\infty)$, one readily infers the following[2]:

$$\mathrm{Res}_1\Big|_{s=-1/2}\zeta_1(s) = \frac{1}{2}\,\tilde{p}_0\;, \tag{46}$$

$$\mathrm{Res}_0\Big|_{s=-1/2}\zeta_1(s) = -\tilde{p}_0\,\log v_0 + \int_0^{v_0} dv\;v\;e_1(v) + \int_{v_0}^{+\infty} dv\;v\left(e_1(v) - \frac{\tilde{p}_0}{v^2}\right). \tag{47}$$

Summing up, Eqs. (44)–(47) give the explicit expression for the renormalized Casimir energy

$$\mathscr{E}(\beta) = \tag{48}$$

$$\frac{1}{2}\left[\Big(1 - \log(2\ell\,v_0)\Big)\tilde{p}_0 + \int_0^{v_0} dv\;v\;e_1(v) + \int_{v_0}^{+\infty} dv\;v\left(e_1(v) - \frac{\tilde{p}_0}{v^2}\right) + \int_0^{+\infty} dv\;\frac{2\,v\;e_1(v)}{e^{\beta v} - 1}\right],$$

where the relative spectral measure $e_1(v)$ and the coefficient $\tilde{p}_0$ are given, respectively, by Eqs. (26)–(27) and Eqs. (29) and (32).

Before proceeding, let us remark that the first three terms in Eq. (48) correspond to the zero temperature ($\beta \to +\infty$) contribution, while the last term gives the temperature correction.

[2]Following [36], for any $s_0 \in \mathbf{C}$ we use the notation

$$\mathrm{Res}_n\Big|_{s=s_0}\zeta_1(s) := \left\{\begin{array}{c}\text{coefficient of } (s-s_0)^{-n} \\ \text{in the Laurent expansion of } \zeta_1(s) \text{ at } s = s_0\end{array}\right\}\;.$$

4.1 The Casimir Energy for a Simple Model in Spatial Dimension d = 3

As a simple application of the results derived previously, let us consider the 3-dimensional configuration corresponding to the choice

$$\alpha(\rho) = \alpha_0 \; \chi_{(0,K^2)}(\rho) \quad \text{for some } \alpha_0, K > 0 \qquad (d = 3)\;;$$

this clearly fulfils our assumptions on α. In the following, in agreement with Eq. (18), we put

$$\tilde{\alpha}_0 := \alpha_0/2\;. \tag{49}$$

In this case, one can derive a simple, fully explicit expression for the corresponding thermal Casimir energy. To this purpose, let us first notice that the expression (27) of the integral I_α can be evaluated to give

$$I_\alpha(\lambda) = \frac{2}{\pi}\left[\arctan\left(\frac{\sqrt{\lambda}}{\tilde{\alpha}_0}\right) - \chi_{(K^2,+\infty)}(\lambda)\;\arctan\left(\frac{\sqrt{\lambda - K^2}}{\alpha_0}\right)\right].$$

Substituting the above result in Eq. (26) and making a few elementary manipulations, one obtains for the relative spectral measure

$$e_1(v) = -\frac{v}{2\pi^2}\left[\arctan\left(\frac{\tilde{\alpha}_0}{v}\right) - \arctan\left(\frac{\tilde{\alpha}_0}{\sqrt{v^2 - K^2}}\right)\chi_{(K,+\infty)}(v)\right],$$

On the other hand, Eqs. (29) and (32) give straightforwardly

$$\tilde{p}_0 = \frac{1}{4\pi^2}\,\tilde{\alpha}_0\;K^2\;.$$

Due to the above results and upon evaluation of some elementary integrals, for any $\beta, \ell \in (0,+\infty)$ and some fixed $v_0 \in (0, K)$ chosen arbitrarily, Eq. (48) yields

$$\mathscr{E}(\beta) = -\frac{1}{12\pi^2}\left[\frac{\pi}{2}K^3 + \frac{3}{2}\,\tilde{\alpha}_0\,K^2\left(\log(\ell\,R) - \frac{7}{6}\right) + \tilde{\alpha}_0^3\;\log\left(\frac{2\tilde{\alpha}_0}{K}\right) - \omega(\tilde{\alpha}_0, K) + \right.$$
$$\left. + \int_0^{+\infty} dv\left(\frac{6\,v^2}{e^{\beta v} - 1} - \frac{6\,v\,\sqrt{v^2 + K^2}}{e^{\beta\sqrt{v^2+K^2}} - 1}\right)\arctan\left(\frac{\tilde{\alpha}_0}{v}\right)\right],$$

where we have introduced the (continuous) function

$$\omega(x,y) := \begin{cases} (x^2-y^2)^{3/2}\,\mathrm{arccoth}\left(\dfrac{x}{\sqrt{x^2-y^2}}\right) & \text{for } x \geq y\,, \\ (y^2-x^2)^{3/2}\left[\dfrac{3\pi}{2} - \arctan\left(\dfrac{x}{\sqrt{y^2-x^2}}\right)\right] & \text{for } x < y\,. \end{cases}$$

Note that the above result allows to infer by simple arguments that, in the limiting case where α_0 is kept fixed and $K \to +\infty$, there holds

$$\mathscr{E}(\beta) = \frac{\tilde{\alpha}_0^3}{12\pi^2}\Bigg[\pi\,\frac{K^3}{\tilde{\alpha}_0^3} - \frac{3}{2}\,\frac{K^2}{\tilde{\alpha}_0^2}\left(\log(\ell\,K) - \frac{1}{2}\right) - \frac{9\pi}{4}\,\frac{K}{\tilde{\alpha}_0} + \log(\ell K) + \\ + \left(\frac{4}{3} - \log(2\ell\tilde{\alpha}_0)\right) - \frac{1}{\tilde{\alpha}_0^3}\int_0^{+\infty} dv\,\frac{6\,v^2}{e^{\beta v}-1}\,\arctan\left(\frac{\tilde{\alpha}_0}{v}\right) + O\left(\frac{\tilde{\alpha}_0}{K}\right)\Bigg]\,. \tag{50}$$

Obviously enough, the above result allows to make a comparison with the model corresponding to a constant, not compactly supported function

$$\alpha(\rho) = \alpha_0 \quad \text{for all } \rho \in [0,+\infty) \text{ and some } \alpha_0 > 0 \qquad (d=3)\,, \tag{51}$$

that is the model typically considered in the literature [5, 19, 22, 23, 30]; as reviewed in Appendix, in this case the Casimir energy is given by

$$\mathscr{E}(\beta) = \frac{\tilde{\alpha}_0^3}{12\pi^2}\left(\frac{4}{3} - \log(2\ell\tilde{\alpha}_0)\right) - \frac{1}{2\pi^2}\int_0^{+\infty} dv\,\frac{v^2}{e^{\beta v}-1}\,\arctan\left(\frac{\tilde{\alpha}_0}{v}\right)\,. \tag{52}$$

This appears to coincide with the finite, "renormalized" part of the asymptotic expansion (50), which is obtained removing by brute force the divergent terms in the cited expansion.

Acknowledgements C.C. and D.F. acknowledge the support of the FIR 2013 project "Condensed Matter in Mathematical Physics", Ministry of University and Research of Italian Republic (code RBFR13WAET).

Appendix: The Case $\alpha = const.$ in Spatial Dimensions $d = 3$

In order to make connection with the existing literature, in the present appendix we briefly review the computation of the Casimir energy for the 3-dimensional model described in Eq. (51), that is

$$\alpha(\rho) = \alpha_0 \quad \text{for all } \rho \in [0,+\infty) \text{ and some } \alpha_0 > 0 \qquad (d=3)\,.$$

As a matter of fact, it can be easily checked that all the arguments described in the present manuscript continue to make sense also in this particular case, even though α does not fulfil the required assumptions since it does not have compact support.

First of all, let us notice that the integral representation (20) for the function $r_1(z)$ continues to make sense for any $z \in \mathbf{C} \setminus [0, +\infty)$ (the integral in the cited equation is trivially seen to remain finite in the present case). Then, by the same arguments of Sect. 3.1 one obtains an expression like Eq. (26) for the relative spectral measure $e_1(v)$; moreover, the term I_α appearing therein (given by Eq. (27)) can be evaluated explicitly. This allows to infer for the relative spectral measure the expression

$$e_1(v) = -\frac{v}{2\pi^2}\ \arctan\left(\frac{\tilde{\alpha}_0}{v}\right)\ \chi_{(0,+\infty)}(v)\ , \tag{53}$$

where $\tilde{\alpha}_0$ is defined according to Eq. (49). This shows that the map $v \mapsto e_1(v)$ is continuous on $(0, +\infty)$ and fulfils, for any $N \in \{0, 1, 2, \ldots\}$,

$$e_1(v) = \begin{cases} O(v) & \text{for } v \to 0^+\ , \\ \displaystyle\sum_{n=0}^{N} \frac{(-1)^{n+1}\, \tilde{\alpha}_0^{2n+1}}{2\pi^2(2n+1)}\ v^{-2n} + O(v^{-2(N+1)}) & \text{for } v \to +\infty\ . \end{cases}$$

Next, let us consider the representation (16) of the relative zeta function $\zeta_1(s)$ in terms of $e_1(v)$; in view of the above considerations, it appears that the integral in the cited equation is finite for any complex s inside the strip

$$\left\{ s \in \mathbf{C}\ \middle|\ \frac{1}{2} < \mathrm{Re}\ s < 1 \right\}.$$

To proceed, notice that for any such s the integral in Eq. (16) can be evaluated explicitly using the expression (53) for $e_1(v)$; one obtains

$$\zeta_1(s) = -\frac{\tilde{\alpha}_0^{2-2s}}{8\pi\ (s-1)\ \cos(\pi s)}\ ,$$

which determines the analytic continuation of $s \mapsto \zeta_1(s)$ to a function which is meromorphic on the whole complex plane, with simple pole singularities at $s = 1$ and $s = \pm 1/2, \pm 3/2, \ldots$.

Using the above expression for $\zeta_1(s)$ and Eqs. (44)–(45) for the thermal Casimir energy $\mathscr{E}(\beta)$, one easily infers the final result (52), that is

$$\mathscr{E}(\beta) = \frac{\tilde{\alpha}_0^3}{12\pi^2}\left(\frac{4}{3} - \log(2\ell\tilde{\alpha}_0)\right) - \frac{1}{2\pi^2}\int_0^{+\infty} dv\ \frac{v^2}{e^{\beta v} - 1}\ \arctan\left(\frac{\tilde{\alpha}_0}{v}\right).$$

For completeness, let us mention that the above expression can be easily employed to derive the zero temperature expansion ($\beta \to +\infty$) of the Casimir energy $\mathscr{E}(\beta)$.

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Analysis of Fluctuations Around Non-linear Effective Dynamics

Serena Cenatiempo

Abstract We consider the derivation of effective equations approximating the many-body quantum dynamics of a large system of N bosons in three dimensions, interacting through a two-body potential $N^{3\beta-1}V(N^{\beta}x)$. For any $0 \leq \beta \leq 1$ well known results establish the trace norm convergence of the k-particle reduced density matrices associated with the solution of the many-body Schrödinger equation towards products of solutions of a one-particle non linear Schrödinger equation, as $N \to \infty$. In collaboration with C. Boccato and B. Schlein we studied fluctuations around the approximate non linear Schrödinger dynamics, obtaining for all $0 < \beta < 1$ a norm approximation of the evolution of an appropriate class of data on the Fock space.

Keywords Gross-Pitaevskii equation • Interacting bosons • Nonlinear Schrödinger equations • Quantum dynamics • Quantum fluctuations

1 Introduction

The understanding of the properties of many body quantum systems is a challenging topic in quantum mechanics, the challenge being how to derive from the microscopic and fundamental description of the system those collective properties which are successfully exploited in condensed matter laboratories. The analysis of the time evolution of quantum many particle systems and the derivation of effective descriptions in interesting limiting regimes nestle in this research line. From a mathematical physics perspective the main goals in this field are on the one hand to justify the use of effective equations, and on the other hand to clarify the limits of applicability of the effective theories.

While we refer to [5] for an introduction on this topic, and a panorama on existing results and open problems in the context of bosonic and fermionic systems, we focus

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A. Michelangeli, G. Dell'Antonio (eds.), *Advances in Quantum Mechanics*,
Springer INdAM Series 18, DOI 10.1007/978-3-319-58904-6_6

here on some recent results concerning the analysis of the time evolution of bosonic systems in three dimensions.

A bosonic system of N particles moving in three space dimensions can be described through a complex-valued wave function ψ_N on the Hilbert space of permutation symmetric $L^2(\mathbb{R}^{3N})$ wave functions

$$L^2_s(\mathbb{R}^{3N}) = \{ \ \psi_N \in L^2(\mathbb{R}^{3N}) : \psi_N(x_{\pi(1)}, \ldots, x_{\pi(N)}) = \psi_N(x_1, \ldots, x_N) \text{ for any permutation } \pi \in S_N\}$$

with $\|\psi_N\|_2 = 1$. The evolution of an initial wave function $\psi_{N,0} \in L^2_s(\mathbb{R}^{3N})$ is governed by the Schrödinger equation

$$i\partial_t \psi_{N,t} = H_N \psi_{N,t} , \tag{1}$$

where the subscript t indicates the time dependence of $\psi_{N,t}$ and H_N is a self adjoint operator on $L^2_s(\mathbb{R}^{3N})$ known as Hamiltonian of the system. We will restrict our attention to Hamiltonians with two body interactions, and we will consider interactions scaling with the number of particles, as follows:

$$H_N^{(\beta)} = \sum_{i=1}^{N} (-\Delta_{x_i}) + \sum_{i<j}^{N} N^{3\beta-1} V(N^\beta(x_i - x_j)) , \tag{2}$$

with $0 \le \beta \le 1$ and V a spherically symmetric interaction potential. We will be interested in situations where the number of particles N is large.

For $\beta = 0$ the Hamiltonian (2) describes N bosons interacting by a mean field potential $N^{-1}V(x_i - x_j)$; this regime is a first approximation for the behaviour of dilute Bose gases and is characterized by very weak interactions for large N. A more accurate model for interactions among bosons in experiments on cold gases is given by the so called *Gross-Pitaevskii regime*, which corresponds to the $\beta = 1$ case in (2). In this regime the interaction scales as $N^2 V(N(x_i - x_j))$, corresponding to a situation where there are strong and short range collisions. While in the mean field regime, as we will see, correlations among particles can be neglected in order to obtain a (first) effective description of the system, they play a crucial role in the Gross-Pitaevskii regime, due to the singularity of the potential. Values of β between zero and one describe intermediate scalings between the mean field and Gross-Pitaevskii regimes, and therefore we may expect correlations to become more and more important as β approaches one.

We will be interested in studying the evolution under (2) of a particular class of initial data, exhibiting *complete condensation*, meaning that there exists a one-particle wave function $\varphi \in L^2(\mathbb{R}^3)$ (the so called *condensate wave function*) such that the one-particle reduced density matrix associated to the many body wave function $\psi_{N,0}$

$$\gamma^{(1)}_{N,0} := N\mathrm{Tr}_{2\ldots N} |\psi_{N,0}\rangle\langle\psi_{N,0}| , \tag{3}$$

satisfies

$$\mathrm{Tr}\Big| N^{-1}\gamma^{(1)}_{N,0} - |\varphi\rangle\langle\varphi| \Big| \to 0 \qquad \text{as } N \to \infty\,, \tag{4}$$

where $|\varphi\rangle\langle\varphi|$ denotes the orthogonal projection onto φ. From a physical point of view bosonic quantum states such that the one-particle reduced density matrix has an eigenvalue of order N in the limit of large N are models for *Bose-Einstein condensates*, as realized in experiments on low density cold gases since 20 years [1].

We recall that the expectation of a bounded one particle observable $O^{(1)}$ on the many particle state described by $\psi_{N,0}$ is given by $\mathrm{Tr}(\gamma^{(1)}_{N,0}O^{(1)})$. Therefore whenever (4) occurs the knowledge of the condensate wave function is sufficient to determine the expectation of any bounded observable on the state described by $\psi_{N,0}$ in the limit $N \to \infty$. Additionally, since property (4) for bosonic systems also implies that for any $k = 2, 3, \ldots, N$ the k-particle reduced density matrix $\gamma^{(k)}_{N,0} = \binom{N}{k}\mathrm{Tr}_{k+1,\ldots,N}|\psi_{N,0}\rangle\langle\psi_{N,0}|$ is given by a rank one projection onto $\binom{N}{K}\varphi^{\otimes k}$, we can also calculate the expectation of *any* bounded k-particle observable in the limit $N \to \infty$.

Now, let us start with an initial datum satisfying (4) and let the system evolve with the Hamiltonian (2). Due to the presence of the interaction we cannot expect (4) to hold at positive times. However one can show that this property remains approximately true in the limit of large N. Furthermore, one can derive an effective dynamics for the condensate wave function in the scaling regimes described by (2). More precisely one can prove (references will follow at the end of this section) that, for every family of initial data $\psi_{N,0} \in L^2(\mathbb{R}^{3N})$ satisfying (4), the one-particle reduced density matrix $\gamma^{(1)}_{N,t}$ corresponding to the evolved state $\psi_{N,t} = e^{-itH^{(\beta)}_N}\psi_{N,0}$ (under suitable assumptions on the interacting potential) satisfies

$$\mathrm{Tr}\big|N^{-1}\gamma^{(1)}_{N,t} - |\varphi_t\rangle\langle\varphi_t|\big| \xrightarrow[N\to\infty]{} 0\,, \tag{5}$$

with φ_t solution of a non linear Schrödinger equation with initial datum $\varphi_0 = \varphi$, whose precise form depends on β. In particular φ_t satisfies:

$$i\partial_t\varphi_t = -\Delta\varphi_t + (V \star |\varphi_t|^2)\varphi_t \qquad \text{if } \beta = 0\,, \tag{6}$$

$$i\partial_t\varphi_t = -\Delta\varphi_t + (\int V)\,|\varphi_t|^2\varphi_t \qquad \text{if } 0 < \beta < 1\,, \tag{7}$$

$$i\partial_t\varphi_t = -\Delta\varphi_t + 8\pi a_0|\varphi_t|^2\varphi_t \qquad \text{if } \beta = 1\,. \tag{8}$$

The parameter a_0 appearing in (8) is the scattering length of the interaction V, *i.e.* $8\pi a_0 = \int V(x)f(x)$ with $f(x)$ the solution of the zero energy scattering equation

$$\Big(-\Delta + \frac{1}{2}V\Big)f = 0\,, \qquad f(x) \xrightarrow[x\to\infty]{} 1\,. \tag{9}$$

From a physical point of view the scattering length a_0 describes the low-energy scattering among particles, in the sense that two particles interacting through the potential V, when they are far apart, feel the other particle as a hard sphere with radius a_0.

The appearance of a_0 in the effective equation (8) is a consequence of the fact that the many body Schrödinger evolution with Gross-Pitaevskii potential develops a singular correlation structure which varies on the same length scale of the potential. Heuristically this can be seen considering the evolution equation for the one-particle reduced density matrix

$$i\partial_t \gamma^{(1)}_{N,t} = [-\Delta, \gamma^{(1)}_{N,t}] + \frac{1}{2}\mathrm{Tr}_2\big[V_N(x_1 - x_2), \gamma^{(2)}_{N,t}\big]\,. \tag{10}$$

To take into account correlations among the particles and the short scale structure they create in the marginal density $\gamma^{(2)}_{N,t}$, we may use the ansatz

$$\begin{aligned} N^{-1}\gamma^{(1)}_{N,t}(x_1; x_1') &= \varphi_t(x_1)\varphi_t(x_1')\,, \\ \binom{N}{2}^{-1} \gamma^{(2)}_{N,t}(x_1, x_2; x_1', x_2') &= f_N(x_1 - x_2) f_N(x_1' - x_2')\varphi_t(x_1)\varphi_t(x_2)\varphi_t(x_1')\varphi_t(x_2')\,, \end{aligned} \tag{11}$$

with $f_N(x) = f(Nx)$ the zero energy scattering function corresponding to the potential $N^2 V(Nx)$. Then Eq. (8) arises from (10) as the self consistent equation for φ_t; the coefficient in front of the non linearity is given by $\int \mathrm{d}x N^3 V(N(x)) f(Nx) = 8\pi a_0$. Note that the ansatz (11) does not contradict complete condensation of the system at time t. On the contrary in the weak limit $N \to \infty$ the function f_N converges to one, and therefore $\gamma^{(2)}_{N,t}$ converges to $|\varphi_t\rangle\langle\varphi_t|^{\otimes 2}$.

This heuristics also explains why for $0 < \beta < 1$ we get $\int V$ instead of a_0 in the effective equation for φ_t, starting from the ansatz (11). As shown for example in [7, Lemma 2.1] the potential $N^{3\beta-1}V(N^\beta x)$ has scattering length of order N^{-1} for any choice of $0 < \beta < 1$, and the solution $f_{N^\beta}(x)$ of the scattering equation with potential $N^{3\beta-1}V(N^\beta x)$ satisfies the bound

$$\big(1 - f_{N^\beta}\big)(x) \leq \frac{C}{N(|x| + N^{-\beta})} \qquad \text{for } 0 < \beta < 1\,. \tag{12}$$

Therefore the coefficient appearing in front of the non linearity in the self consistent equation for φ_t, obtained from (10) under the assumptions (11) with $f_N(x)$ substituted by $f_{N^\beta}(x)$, is

$$\int \mathrm{d}x\, N^{3\beta} V(N^\beta x) f_{N^\beta}(x) = \int V - cN^{\beta-1}\,, \tag{13}$$

which equals $\int V$ in the limit $N \to \infty$, for any $0 < \beta < 1$. Thus $\beta = 1$ is the only scaling for which the coefficient of the non linearity in the effective equation for φ_t is given by the scattering length of the unscaled potential V.

The rigourous derivation of the effective equation (6) (the *Hartree equation*), in the form presented in (5), has been first obtained by Spohn [36] for bounded potentials, and Erdős-Yau [2, 11] for singular potentials, analysing the BBGKY hierarchy for the density matrices. More recent approaches by Rodnianskii-Schlein [34] and Knowles-Pickl [23] also give the rate of convergence towards the Hartree dynamics. A derivation of the *Gross-Pitaevskii equation* (8) was obtained in a series of works [12, 14, 15] and later with an alternative approach in [30]. More recently, convergence towards the Gross-Pitaevskii dynamics with a precise rate of convergence has been obtained in [4]. The derivation of the non linear Schrödinger equation in the intermediate regimes $0 < \beta < 1$ may be obtained with the same approaches, and it is in fact a simpler problem than the $\beta = 1$ case (see for example [13, 30]; the proof in [4] could be also easily adapted to cover any $\beta < 1$).

Beyond the approximation for the reduced density matrices, there is some interest in obtaining an approximation for the evolved N-particle wave function $\psi_{N,t}$ in the appropriate Hilbert space norm. This corresponds to study fluctuations around the effective dynamics described by the non linear Schrödinger equation for the condensate wave function. Several results in this direction have been obtained in the mean field regime, starting from the pioneering works by Hepp and Ginibre-Velo [16, 22] and later in [3, 8, 9, 20, 21, 26, 27]. More recent results deal with the intermediate scalings with $\beta > 0$, see [7, 18, 19, 28, 29]. In particular, the result in [7] covers all $\beta < 1$. An analogous result for the Gross-Pitaevskii regime is up to now still open.

More generally, from a statical point of view, one would aim to completely construct the ground state wave function and study its excitation spectrum at least in the interesting limiting regimes described by (2) (and even more ambitiously in the thermodynamic limit). These goals have been partially achieved in the context of mean field bosons, where the ground state energy and excitation spectrum have been proved to be correctly described by the famous Bogoliubov approximation [10, 17, 25, 35] and the ground state has been fully constructed in the presence of an ultraviolet cutoff [31–33]. Up to now no similar results are available for any $\beta > 0$.[1] From this point of view studying the fluctuation dynamics for $\beta > 0$ may also give some insight into the problem of approximating the ground state.

The aim of this contribution is to present the strategy used in [7] to obtain a norm approximation for the dynamics described by the Hamiltonian $H_N^{(\beta)}$, with $0 < \beta < 1$. This approximation is obtained for a special class of initial data in the Fock space. The choice of the initial data is a main point in our analysis, since in order to cover all $\beta < 1$ we need to introduce a suitable correlation structure among particles. We will come back to the role of correlations in our analysis in the next sections.

[1]Very recently, after the submission of this contribution, the validity of Bogoliubov prediction for the ground state energy and the low-lying excitation spectrum has been established for any $\beta > 0$ [6].

2 The Coherent State Approach

The strategy used in [7], also known as *coherent state approach*, was first introduced by Hepp in [22]. More recently it has been further developed in [34] and [4] to obtain the rate of the trace norm convergence in the mean field and Gross-Pitaevskii regimes respectively. The main idea of this approach is that even if the dynamics described by $H_N^{(\beta)}$ preserves the particle number, it is convenient to represent our bosonic system in the Fock space, where we have the opportunity to consider a more general class of initial data than wave functions in $L^2_s(\mathbb{R}^{3N})$. The choice of the class of initial data crucially depends on the scaling of the potential. For this reason we first describe which choice turns out to be convenient in the mean field regime, and then present the physical and mathematical motivations leading to a different choice in the Gross-Pitaevskii regime. Before that, let us start with summarising the Fock space representation of a bosonic system.

Fock Space Representation

We represent our bosonic system in the bosonic Fock space

$$\mathscr{F} = \oplus_{n\geq 0} L^2_s(\mathbb{R}^{3n}) \,. \tag{14}$$

A state $\Psi \in \mathscr{F}$ is therefore a sequence $\Psi = \{\psi^{(n)}\}_{n\geq 0}$, where $\psi^{(0)} \in \mathbb{C}$ and $\psi^{(n)} \in L^2_s(\mathbb{R}^{3n})$. The space $\mathscr{F}$ is a Hilbert space with respect to the inner product

$$\langle \Psi, \Phi\rangle = \overline{\psi^{(0)}}\varphi^{(0)} + \sum_{n\geq 1} \langle \psi^{(n)}, \varphi^{(n)}\rangle, \tag{15}$$

and each component of $\Psi \in \mathscr{F}$ has a probabilistic interpretation, namely $\|\psi^{(n)}\|_2^2$ is the probability of having n particle in the state described by ψ. Clearly we are interested in states where $\sum_{n\geq 0} \|\psi^{(n)}\|_2^2 = 1$. The number of particles operator is defined requiring that

$$(\mathscr{N}\Psi)^{(n)} = n\psi^{(n)} \,, \tag{16}$$

and therefore the expected number of particles in a state $\Psi \in \mathscr{F}$ is given by

$$\langle \Psi, \mathscr{N}\Psi\rangle = \sum_{n\geq 0} n\|\psi^{(n)}\|_2^2 \,. \tag{17}$$

A state with exactly N particles is represented by a vector in $\mathscr{F}$ where only the N-th component is non zero. A special example of such a state is the vacuum state with $\Omega = \{1, 0, 0, \ldots, 0\}$, describing a state with no particles. More in general, given a one-particle operator $O^{(1)}$ the corresponding operator $d\Gamma(O^{(1)})$ on $\mathscr{F}$ (called *the second quantization* of $O^{(1)}$) is defined by the requirement that

$$\big(d\Gamma(O^{(1)})\Psi\big)^{(n)} = \sum_{i=1}^{n} O_i^{(1)}\psi^{(n)}, \tag{18}$$

where $O_i^{(1)}$ denotes the operator acting on $L^2(\mathbb{R}^{3n})$ as $O^{(1)}$ on the i-th particle and as the identity on the other $(n-1)$ particles.

In order to define a time evolution on $\mathscr{F}$ we introduce the Hamilton operator $\mathscr{H}_N^{(\beta)}$, which is defined through its action on vectors of $\mathscr{F}$:

$$\begin{aligned}(\mathscr{H}_N^{(\beta)}\Psi)^{(n)} &= \big(H_N^{(\beta)}\big)^{(n)}\psi^{(n)}, \\ \big(H_N^{(\beta)}\big)^{(n)} &= \sum_{i=1}^{n}(-\Delta_{x_i}) + \sum_{i<j}^{n} N^{3\beta-1}V(N^{\beta}(x_i-x_j)). \end{aligned} \tag{19}$$

By definition the operator $\mathscr{H}_N^{(\beta)}$ acts on states with a variable number of particles but leaves all sectors with fixed number of particles invariant. Note that the scaling parameter N in $\mathscr{H}_N^{(\beta)}$ in general has nothing to do with the number of particles of the system (which is not fixed now). To recover the relevant scaling limits we are interested in, we will consider in the following the evolution of states with expected number of particle N.

Being the number of particles in $\mathscr{F}$ not fixed, it is useful to introduce operators that create or annihilate a particle. For $f \in L^2(\mathbb{R}^3)$ we define the creation operator $a^*(f)$ and the annihilation operator $a(f)$ by

$$\big(a^*(f)\Psi\big)^{(n)}(x_1,\dots,x_n) = \frac{1}{\sqrt{n}}\sum_{j=1}^{n} f(x_j)\psi^{(n-1)}(x_1,\dots,\not{x}_j,\dots,x_n) \quad n\geq 1, \tag{20}$$

$$\big(a(f)\Psi\big)^{(n)}(x_1,\dots,x_n) = \sqrt{n+1}\int \mathrm{d}x\,\overline{f(x)}\psi^{(n+1)}(x,x_1,\dots,x_n) \qquad n\geq 0, \tag{21}$$

and we set $(a^*(f)\Psi)^{(0)} := 0$. It is simply to check that $a^*(f) = (a(f))^*$, and that the following commutation relations hold:

$$[a(f),a^*(g)] = \langle f,g\rangle_{L^2}, \qquad [a(f),a(g)] = [a^*(f),a^*(g)] = 0. \tag{22}$$

We have $a(f)\Omega = 0$. The action of $(a^*(f))^N$ on the vacuum generates a state with exactly N particles with wave function f, that is

$$(\sqrt{N!})^{-1}(a^*(f))^N = \{0,\dots,0,f^{\otimes N},0,\dots\}. \tag{23}$$

We also introduce operator valued distribution a_x^* and a_x, defined by

$$a^*(f) = \int \mathrm{d}x\, f(x) a_x^* \,, \qquad \text{and} \qquad a(f) = \int \mathrm{d}x\, \overline{f(x)} a_x \,, \tag{24}$$

which formally creates or annihilates a particle in the point x. From (22) we have $[a_x, a_y^*] = \delta_{x,y}$ and $[a_x, a_y] = [a_x^*, a_y^*]$=0.

The second quantization of any (densely defined) self adjoint operator can be conveniently expressed by means of a_x^* and a_x, see e.g. [5, Sect. 3] and [24, Sect. 1.3]. The expressions for the particle number operator and the Hamiltonian are

$$\mathscr{N} = \int \mathrm{d}x a_x^* a_x \,, \tag{25}$$

and

$$\mathscr{H}_N^{(\beta)} = \int \mathrm{d}x \nabla_x a_x^* \nabla_x a_x + \frac{1}{2} \int \mathrm{d}x \mathrm{d}y N^{3\beta - 1} V(N^\beta (x - y)) a_x^* a_y^* a_x a_y \tag{26}$$

respectively. The r. h. s. of (25) and (26) should be understood in the sense of forms; for example (25) means that for any $\Psi, \Phi \in \mathscr{F}$ we have $\langle \Psi, \mathscr{N} \Phi \rangle = \int \mathrm{d}x \, \langle a_x \Psi, a_x \Phi \rangle$.

Moreover, the kernel of the one-particle reduced density matrix $\gamma^{(1)}$ associated to the state $\Psi \in \mathscr{F}$ can be expressed as

$$\gamma^{(1)}(x; y) = \langle \Psi, a_x^* a_y \Psi \rangle \,. \tag{27}$$

The expression (25) for $\mathscr{N}$ suggests that, although creation and annihilation operators are unbounded operators, they can be bounded with respect to the square root of the number of particles operator, in the sense that

$$\begin{aligned} \|a(f)\Psi\| &\le \|f\|_2 \|\mathscr{N}^{1/2}\Psi\| \\ \|a^*(f)\Psi\| &\le \|f\|_2 \|(\mathscr{N} + 1)^{1/2}\Psi\| \end{aligned} \tag{28}$$

for all $f \in L^2(\mathbb{R}^3)$, $\Psi \in \mathscr{F}$. Moreover, given a bounded one particle operator $O^{(1)}$ on the $L^2(\mathbb{R}^3)$ space, its second quantization $d\Gamma(O^{(1)})$, although generally unbounded, is bounded with respect to the number of particles operator:

$$|\langle \Psi, d\Gamma(O^{(1)})\Psi \rangle| \le \|O^{(1)}\| \langle \Psi, \mathscr{N}\Psi \rangle, \quad \Psi \in \mathscr{F} \,. \tag{29}$$

Properties (28) and (29) will be essential for our analysis.

2.1 Choice of the Class of Initial States in the Mean Field Regime

Our goal is to study the time evolution under $\mathscr{H}_N^{(\beta)}$ of a suitable class of initial data in $\mathscr{F}$ with expected number of particles N and one-particle reduced density matrix $\gamma_{N,0}^{(1)}$ satisfying (4) for some $\varphi \in L^2(\mathbb{R}^3)$. In the mean field regime $\beta = 0$ a natural choice is to consider as class of initial data the so called *coherent states*.

A coherent state with wave function $f \in L^2(\mathbb{R}^3)$ is a linear combination of states with all possible number of particles, all described by the same wave function f. Such a state is built acting on the vacuum with the so called *Weyl operator*

$$W(f) = \exp(a^*(f) - a(f)) , \tag{30}$$

thus obtaining

$$W(f)\Omega = e^{-\|f\|^2/2} \left\{ 1, f, \frac{f^{\otimes 2}}{\sqrt{2!}}, \ldots, \frac{f^{\otimes n}}{\sqrt{n!}}, \ldots \right\} . \tag{31}$$

The Weyl operator is a unitary operator on $\mathscr{F}$ which acts on the annihilation and creation operators as follows:

$$\begin{aligned} W^*(f)\, a_x\, W(f) &= a_x + f(x) \\ W^*(f)\, a_x^*\, W(f) &= a_x^* + \overline{f(x)} . \end{aligned} \tag{32}$$

Since the expected particle number of the coherent state $W(f)\Omega$ is equal to

$$\left\langle W(f)\Omega, \mathscr{N} W(f)\Omega \right\rangle = \|f\|_2^2 , \tag{33}$$

a coherent state with expected particle number N is given by

$$W(\sqrt{N}\varphi)\Omega , \quad \|\varphi\|_2 = 1 . \tag{34}$$

Using (32) it is also simple to check that the kernel of the one-particle density associated to $W(\sqrt{N}\varphi)\Omega$ is

$$\gamma_N^{(1)}(x, y) = \left\langle W(\sqrt{N}\varphi)\Omega, a_x^* a_y W(\sqrt{N}\varphi)\Omega \right\rangle = N\overline{\varphi(x)}\varphi(y) . \tag{35}$$

For this class of initial data the following theorem was proven in [34], in the mean field regime.

Theorem 1 *Let V be a measurable function, satisfying the operator inequality $V^2(x) \le C(1-\Delta)$ for some $C > 0$ and let $\varphi \in H^1(\mathbb{R}^3)$. Let $\gamma^{(1)}_{N,t}$ be the one-particle reduced density associated with*

$$\Psi_{N,t} = e^{-it\mathscr{H}_N^{(0)}} W(\sqrt{N}\varphi)\Omega \,.$$

Then, there exist constants $D, k > 0$ s.t.

$$\mathrm{Tr}\left|\gamma^{(1)}_{N,t} - N|\varphi_t\rangle\langle\varphi_t|\right| \le De^{k|t|}$$

for all $t \in \mathbb{R}$ and all $N \in \mathbb{N}$, with φ_t satisfying (6) with initial data $\varphi_0 = \varphi$.

Remark 1 Note that the assumptions on V in Theorem 1 include the Coulomb case $V(x) = \pm 1/|x|$.

The strategy to prove Theorem 1 is to define a unitary operator $U_N(t)$ through the requirement:

$$\Psi_{N,t} = e^{-it\mathscr{H}_N^{(0)}} W(\sqrt{N}\varphi)\Omega := W(\sqrt{N}\varphi_t)U_N(t)\Omega \,. \tag{36}$$

Note that if $U_N(t)$ was the identity operator, than the evolution of $W(\sqrt{N}\varphi)\Omega$ under the mean field Hamiltonian would be exactly a coherent state with evolved wave function φ_t. In this sense the vector $U_N(t)\Omega$ is a fluctuation vector and

$$U_N(t) = W^*(\sqrt{N}\varphi_t)e^{-it\mathscr{H}_N^{(0)}} W(\sqrt{N}\varphi) \,. \tag{37}$$

can be interpreted as a fluctuation dynamics. Using the definition (36) we can write the kernel of the one particle reduced density matrix associated to the evolved state $\Psi_{N,t}$ as follows

$$\gamma^{(1)}_{N,t}(x,y) = \left\langle U_N(t)\Omega, W^*(\sqrt{N}\varphi)a^*_x a_y W(\sqrt{N}\varphi)U_N(t)\Omega\right\rangle . \tag{38}$$

For any compact one-particle observable $O^{(1)}$ on $L^2(\mathbb{R}^3)$ one has

$$\begin{aligned} \mathrm{Tr}\, O^{(1)}\Big(\gamma^{(1)}_{N,t} - N|\varphi_t\rangle\langle\varphi_t|\Big) &= \sqrt{N}\left\langle U_N(t)\Omega, [\, a^*(O^{(1)}\varphi_t) + a(O^{(1)}\varphi_t)\,]U_N(t)\Omega\right\rangle \\ &\quad + \left\langle U_N(t)\Omega, d\Gamma(O^{(1)})U_N(t)\Omega\right\rangle , \end{aligned} \tag{39}$$

with $d\Gamma(O^{(1)})$ defined in (18). Using (28) and (29) we have

$$\left|\mathrm{Tr}\, O^{(1)}\Big(\gamma^{(1)}_{N,t} - N|\varphi_t\rangle\langle\varphi_t|\Big)\right| \le \sqrt{N}\,\left\langle U_N(t)\Omega, (\mathscr{N}+1)U_N(t)\Omega\right\rangle . \tag{40}$$

Since the space of trace class operators on $L^2(\mathbb{R}^3)$, equipped with the trace norm, is the dual of the space of compact operators, equipped with the operator norm, the proof of Theorem 1 ends up with controlling the r.h.s. of (40). In particular, to get a bound on the rate of the convergence of the many body evolution towards the mean field dynamics proportional to $\sqrt{N}$ it is enough to show that the number of particles with respect to the fluctuation dynamics $U_N(t)$ grows uniformly in N. To this aim we compute

$$i\partial_t \big\langle U_N(t)\Omega, \mathcal{N} U_N(t)\Omega \big\rangle = \big\langle U_N(t)\Omega, [\mathcal{L}_N^{(0)}(t), \mathcal{N}] U_N(t)\Omega \big\rangle, \tag{41}$$

with

$$\mathcal{L}_N^{(0)}(t) = \big(i\partial_t W^*(\sqrt{N}\varphi_t)\big) W(\sqrt{N}\varphi_t) + W^*(\sqrt{N}\varphi_t) \mathcal{H}_N^{(0)} W(\sqrt{N}\varphi_t) \,. \tag{42}$$

the generator of the fluctuation dynamics $U_N(t)$. In contrast with the original Hamiltonian, $\mathcal{L}_N^{(0)}(t)$ contains terms which do not commute with $\mathcal{N}$. As a consequence, the expectation of $\mathcal{N}$ is not preserved along the evolution of U_N, that is fluctuations are going to grow. However, under the assumption on the regularity of the potential stated in Theorem 1 it can be shown that

$$\pm \, [\mathcal{L}_N^{(0)}(t), \mathcal{N}] \leq C\big(\mathcal{N} + 1\big) \,. \tag{43}$$

Using a Gronwall lemma, we obtain that $\big\langle U_N(t)\Omega, (\mathcal{N}+1) U_N(t)\Omega \big\rangle$ is bounded uniformly in N. The fact that φ_t should satisfy the Hartree equation (6) arises quite naturally, because this is the condition to be imposed in order to cancel some terms of order $\sqrt{N}$ in the generator which are linear in a_x^* and a_x and therefore do not commute with $\mathcal{N}$. Some more work is needed to get the (optimal) rate of convergence in Theorem 1 rather than the factor $\sqrt{N}$ in (40), but this issue is not relevant for the aim of this contribution.

2.2 Choice of the Class of Initial States in the Gross-Pitaevskii Regime

We consider now the Gross-Pitaevskii regime $\beta = 1$. To get the trace norm convergence result in this regime, the initial data (34) has to be suitably modified to take into account correlations among particles, that play now a crucial role. In fact the Gross-Pitaevskii evolution develops singular correlations which are not captured by an approximation given in terms of coherent states.

From the mathematical point of view this reflects into the fact that we cannot approximate the evolution of the class of coherent states (34) under $\mathcal{H}_N^{(GP)} := \mathcal{H}_N^{(1)}$ with a new coherent state with evolved wave function given by the Gross-Pitaevskii equation (8). If we defined the fluctuation dynamics

$$\tilde{U}_N(t) = W^*(\sqrt{N}\varphi_t) e^{-it\mathcal{H}_N^{(GP)}} W(\sqrt{N}\varphi) \,, \tag{44}$$

analogously to what was done in the mean field regime, then the number of fluctuations $\langle \tilde{U}_N(t)\Omega, \mathcal{N}\tilde{U}_N(t)\Omega\rangle$ would grow with N. In fact the generator of the dynamics $\tilde{U}_N(t)$ contains some linear and quadratic terms in the annihilation and creation operators whose commutator with $\mathcal{N}$ cannot be bounded uniformly in N.

The idea used in [4] to implement the appropriate correlation structure in the Fock space is to define the correlation kernel

$$k_t(x,y) = -N\omega(N(x-y)\varphi_t^N(x)\varphi_t^N(y)\,, \tag{45}$$

with $\omega(x) = 1 - f(x)$, $f(x)$ the solution of the zero energy scattering equation (9), and φ_t^N the solution of the following modified Gross-Pitaevskii equation[2]:

$$i\partial_t\varphi_t^N = -\Delta\varphi_t^N + \big(N^3V(N\cdot)f(N\cdot)\star|\varphi_t^N|^2\big)\varphi_t^N\,. \tag{46}$$

It is simple to check that the function $\omega(x)$ satisfies the bound $N\omega(Nx) \le C(|x| + 1/N)^{-1}$ and k_t is the kernel of an Hilbert-Schmidt operator. In the following we identify the function $k_t \in L^2(\mathbb{R}^3\times\mathbb{R}^3)$ with the operator having k_t as its integral kernel. Using k_t we define a unitary operator $T(k_t)$ acting on the Fock space $\mathcal{F}$ by

$$T(k_t) = e^{\frac{1}{2}\int \mathrm{d}x\mathrm{d}y\,(k_t(x,y)a_x^*a_y^* - \bar{k}_t(x,y)a_xa_y)}\,. \tag{47}$$

The action of $T(k_t)$ on the creation and annihilation operators can be explicitly computed. For any $f \in L^2(\mathbb{R}^3)$ we have (see [4, Lemma 2.3])

$$\begin{aligned} T^*(k_t)\,a(f)T(k_t) &= a(\cosh_{k_t}(f)) + a^*(\sinh_{k_t}(\bar{f})) \\ T^*(k_t)\,a^*(f)T(k_t) &= a^*(\cosh_{k_t}(f)) + a(\sinh_{k_t}(\bar{f}))\,, \end{aligned}$$

where we used the notation $\cosh_{k_t}$ and $\sinh_{k_t}$ for the linear operators on $L^2(\mathbb{R}^3)$ given by

$$\cosh_{k_t} = \sum_{n\ge 0}\frac{1}{(2n)!}(k_t\bar{k}_t)^n\,, \qquad \sinh_{k_t} = \sum_{n\ge 0}\frac{1}{(2n+1)!}(k_t\bar{k}_t)^n k_t\,, \tag{48}$$

where products of k_t and $\bar{k}_t$ have to be understood as products of operators. We now use the unitary operator $T(k_t)$ to approximate the correlation structure developed by the many-body evolution. To this aim, we consider the evolution of initial data

[2]The choice of using the solution of the modified Gross-Pitaevskii equation (46) rather than the solution of Eq. (8) is due to technical reasons; however note that in the limit $N \to \infty$ the solution of (46) approaches the solution of (8), as shown in [4, Proposition 3.1]. Despite the operators k_t being N-dependent we do not put an extra N-index to keep the notation light.

having the form

$$\Psi_{N,0} = W(\sqrt{N}\varphi)T(k_0)\Omega \,. \tag{49}$$

Initial data given by Eq. (49), known as *squeezed coherent states*, are a natural class of initial data approximating the ground state of Bose-Einstein condensates trapped in a volume of order one. In fact they have expected particle number $N + \|k_t\|_2$ (with $\|k_t\|$ of order one) and energy equal at leading order to ground state energy for trapped bosons in the Gross-Pitaevskii regime, see [5, Appendix A]. From a physical point of view a good approximation for the ground state energy of a system of N bosons is believed to be of the form $\varphi^{\otimes N}\prod_{i<j} f(N(x_i - x_j))$. Then, the class of states $W(\sqrt{N}\varphi)T(k_0)\Omega \in \mathscr{F}$ captures some of the correlations which are believed to truly appear in the ground state of dilute bosonic systems.

The trace norm convergence result in the Gross-Pitaevskii regime is obtained studying the dynamics of states of the form $\Psi_{N,0} = W(\sqrt{N}\varphi)T(k_0)\Omega$ under the Gross-Pitaevskii Hamiltonian $\mathscr{H}_N^{(GP)}$. The fluctuation operator $\mathscr{U}_N(t)$ is defined through the requirement that the many body evolution preserves the form of the initial data, up for the evolution of φ into φ_t^N, that is

$$\Psi_{N,t} = e^{-it\mathscr{H}_N^{(GP)}} W(\sqrt{N}\varphi)T(k_0)\Omega := W(\sqrt{N}\varphi_t^N)T(k_t)\mathscr{U}_N(t)\Omega \,. \tag{50}$$

If $\mathscr{U}_N(t)$ was the identity operator then the evolution of a state of the form (49) would be a state of the same type with evolved condensate wave function φ_t^N given by the modified Gross-Pitaevskii equation (46). In this sense $\mathscr{U}_N(t)\Omega$ is a fluctuation vector and we refer to $\mathscr{U}_N(t)$ as a fluctuation dynamics. Using the definition (50) we can write the kernel of the one particle reduced density matrix associated to the evolved state $\Psi_{N,t}$ as follows

$$\gamma_{N,t}^{(1)}(x,y) = \left\langle \mathscr{U}_N(t)\Omega, T^*(k_t)W^*(\sqrt{N}\varphi_t^N)a_x^* a_y W(\sqrt{N}\varphi_t^N)T(k_t)\mathscr{U}_N(t)\Omega \right\rangle, \tag{51}$$

with

$$\mathscr{U}_N(t) = T^*(k_t)W^*(\sqrt{N}\varphi_t^N)e^{-it\mathscr{H}_N^{(GP)}} W(\sqrt{N}\varphi)T(k_0)\,. \tag{52}$$

The generator of the fluctuation dynamics $\mathscr{U}_N(t)$ is given by

$$\begin{aligned} \mathscr{L}_N(t) &= (i\partial_t T^*(k_t))T(k_t) \\ &+T^*(k_t)\big[\left(i\partial_t W^*(\sqrt{N}\varphi_t^N)\right) W(\sqrt{N}\varphi_t^N) + W^*(\sqrt{N}\varphi_t^N)\mathscr{H}_N^{(GP)} W(\sqrt{N}\varphi_t^N)\big]T(k_t)\,, \end{aligned} \tag{53}$$

where

$$\begin{aligned} T^*(k_t)W^*(\sqrt{N}\varphi_t^N)a_x W(\sqrt{N}\varphi_t^N)T(k_t) &= \sqrt{N}\,\varphi_t^N(x) + a(c_x) + a^*(s_x) \\ T^*(k_t)W^*(\sqrt{N}\varphi_t^N)a_x^* W(\sqrt{N}\varphi_t^N)T(k_t) &= \sqrt{N}\,\overline{\varphi_t^N(x)} + a^*(c_x) + a(s_x)\,, \end{aligned} \tag{54}$$

with $c_x(z) = \cosh_{k_t}(z,x)$ and $s_x(z) = \sinh_{k_t}(z,x)$. Note that the action of the Bogoliubov transformation $T(k_t)$ in Eq. (53) generates terms in $\mathscr{L}_N(t)$ where the creation and annihilation operators are not in normal order (a product of creation and annihilation operators is said to be normal ordered if all creation operators are to the left of all annihilation operators). When we use the commutation relations (22) to restore the normal order, this procedure generates some new linear and quadratic terms in the creation and annihilation operators, coming from the normal ordering of some cubic and quartic terms respectively. These terms, together with the fact that the correlation kernel k_t contains the solution f_N of the scattering equation, lead to some cancellations in the generator $\mathscr{L}_N$ which are essential to control the growth of the number of fluctuations uniformly in N. In particular, the sum of the linear terms (which would be of order $\sqrt{N}$) gives zero when φ_t^N is chosen to satisfy the effective equation (46). A second cancellation arises between some quadratic terms that are too singular in the Gross-Piteavskii regime. After these cancellations (see [4, Sect. 3] for details) we have

$$\pm\,[\mathscr{L}_N(t), \mathscr{N}] \leq \mathscr{H}_N + c\mathscr{N}^2/N + Ce^{k|t|}\big(\mathscr{N} + 1\big) \tag{55}$$

for some $C, c, k > 0$ independent on N and t. The time dependence on the r.h.s. of the last equation arises through high Sobolev norms of the solution φ_t of the Gross-Pitaevskii equation.

The bound (55) shows a further difference with respect to the strategy used to prove Theorem 1: in order to control the growth of the number of fluctuations $\big\langle \mathscr{U}_N(t)\Omega, \mathscr{N}\mathscr{U}_N(t)\Omega\big\rangle$ in the Gross-Pitaevskii case we also need to control the growth of $\mathscr{H}_N$. To this aim, in a very similar way as used to prove (55) one can also obtain the bounds

$$\mathscr{L}_N(t) \leq \frac{3}{2}\,\mathscr{H}_N + c\mathscr{N}^2/N + ce^{k|t|}(\mathscr{N} + 1)\,, \tag{56}$$

$$\mathscr{L}_N(t) \geq \frac{1}{2}\,\mathscr{H}_N - c\mathscr{N}^2/N - ce^{k|t|}(\mathscr{N} + 1)\,, \tag{57}$$

$$\pm\dot{\mathscr{L}}_N(t) \leq 2\,\mathscr{L}_N(t) + ce^{k|t|}(\mathscr{N} + 1 + \mathscr{N}^2/N)\,. \tag{58}$$

Moreover, it is easy to show that the number of fluctuations is just bounded by the total number of particles:

$$\big\langle \mathscr{U}_N(t)\Omega, (\mathscr{N}^2/N)\mathscr{U}_N(t)\Omega\big\rangle \leq \big\langle \mathscr{U}_N(t)\Omega, \mathscr{N}\mathscr{U}_N(t)\Omega\big\rangle + \big\langle \Omega, (\mathscr{N}^2/N)\,\Omega\big\rangle. \tag{59}$$

Using (55), (56), (58) and (59) one is able to close a Gronwall type estimate for the expectation

$$\big\langle \mathscr{U}_N(t)\Omega, \big(\,\mathscr{L}_N(t) + De^{k|t|}(\mathscr{N} + 1)\big)\mathscr{U}_N(t)\Omega\big\rangle\,, \tag{60}$$

for some $D > 0$, and show that it remains bounded uniformly in N. We get finally the desired bound on the growth of $\mathcal{N}$ observing that the lower bound (57) together with (59) implies

$$\left\langle U_N(t)\Omega, \left(2\mathcal{L}_N(t) + c_1 e^{k|t|}(\mathcal{N}+1)\right) U_N(t)\Omega \right\rangle \geq \left\langle U_N(t)\Omega, \mathcal{H}_N U_N(t)\Omega \right\rangle \geq 0\,,$$

for some $c_1 > 0$. Since D can be chosen to be greater than $(c_1 + 1)$, the bound for (60) also implies that $\left\langle U_N(t)\Omega, \mathcal{N}\, U_N(t)\Omega \right\rangle$ remains bounded uniformly in N. This allows to prove the following theorem, see [4].

Theorem 2 *Consider a non-negative and spherically symmetric potential $V \in L^1 \cap L^3(\mathbb{R}^3, (1+|x|^6)dx)$. Let $\varphi \in H^4(\mathbb{R}^3)$ and $\Omega \in \mathcal{F}$ the vacuum state. Consider the family of initial data*

$$\Psi_N = W(\sqrt{N}\varphi)T(k_0)\Omega\,,$$

and denote by $\gamma^{(1)}_{N,t}$ the one-particle reduced density matrix associated with the evolution $\Psi_{N,t} = e^{-it\mathcal{H}_N^{(GP)}}\Psi_N$. Then

$$\operatorname{Tr}\left|\gamma^{(1)}_{N,t} - N|\varphi_t\rangle\langle\varphi_t|\right| \leq CN^{1/2}\exp(\exp(c|t|))$$

for all $t \in \mathbb{R}$. Here φ_t satisfies the Gross-Pitaevskii equation (8) .

Remark 2 Theorem 2 still holds if we substitute the vacuum state Ω with a sequence of states $\xi_N \in \mathcal{F}$ such that $\|\xi_N\| = 1$ and $\left\langle \xi_N, \left(\mathcal{H}_N^{(GP)} + \mathcal{N} + \mathcal{N}^2/N\right)\xi_N \right\rangle \leq C$, for some $C > 0$ independent on N.

3 Norm Approximation Result and Ideas of the Proof

We switch now to the problem of studying fluctuations around the effective dynamics described by (6), (7) or (8). The fact that the coherent state approach could also be used to describe fluctuations around the limiting equation has been first exploited in [16, 22, 34] in the mean field setting.

In [7] we follow the strategy used in [34], the main difference coming from the necessity of taking into account correlations among particles in the condensate. As discussed in the introduction, the many body evolution given by $\mathcal{H}_N^{(\beta)}$ for $0 < \beta < 1$ develops weaker correlations than in the Gross-Pitaevskii regime. This is the reason why the effective dynamics is described by the non linear Schrödinger equation (7), rather than the Gross-Pitaevskii equation (8). Anyway two body correlations are not negligible in the analysis of fluctuations. In fact, to get a norm approximation result valid for all $\beta < 1$, we need to introduce a correlation structure, which is a suitable modification of the one defined in (45). More precisely, instead of working with the kernel defined in (45) we consider

$$k_{\ell,t}(x;y) = -N\omega_{N,\ell}(x-y)(\tilde{\varphi}_t^N((x+y)/2))^2 \,. \tag{61}$$

Here $\tilde{\varphi}_t^N$ is the solution of the N-dependent Schrödinger equation

$$i\partial_t\tilde{\varphi}_t^N = -\Delta\tilde{\varphi}_t^N + \big(N^{3\beta}V(N^\beta\cdot)f_{N,\ell}\star|\tilde{\varphi}_t^N|^2\big)\tilde{\varphi}_t^N \,, \tag{62}$$

$\omega_{N,\ell} = 1-f_{N,\ell}$, and $f_{N,\ell}$ is the solution of the eigenvalue problem

$$\Big[-\Delta + \frac{1}{2}N^{3\beta-1}V(N^\beta x)\Big]f_{N,\ell}(x) = \lambda_{N,\ell}\, f_{N,\ell}(x)\chi(|x|\leq\ell) \,, \tag{63}$$

associated with the smallest possible eigenvalue $\lambda_{N,\ell}$, normalized so that $f_{N,\ell} = 1$ for $|x| = \ell$ and continued to $\mathbb{R}^3$ by requiring that $f_{N,\ell} = 1$ for all $|x| \geq \ell$. With this choice the kernel $k_{\ell,t}(x;y) = 0$ for all $|x-y| > \ell$, that is we are considering particles correlated up to relative distance ℓ. Note that, for all $0 < \beta < 1$, the solution $\tilde{\varphi}_t^N$ of (62) approaches the solution of the non linear equation (7) as $N \to \infty$. However it furnishes a better approximation for the dynamics of the condensate wave function, since it contains the factor $f_{N,\ell}$ which takes into account the correlations among the particles.

Using $k_{\ell,t}$ we define the Bogoliubov transformation $T(k_{\ell,t})$ through (47). For any $0 < \beta < 1$ we consider the evolution of initial data of the form $W(\sqrt{N}\varphi)T(k_{\ell,0})\Omega$, defining the fluctuation dynamics:

$$\mathscr{U}_{\ell,N}(t) = T^*(k_{\ell,t})W^*(\sqrt{N}\tilde{\varphi}_t^N)e^{-it\mathscr{H}_N^{(\beta)}}W(\sqrt{N}\varphi)T(k_{\ell,0}) \,, \tag{64}$$

with $\tilde{\varphi}_0^N = \varphi$. The following result holds.

Theorem 3 *Let $V \geq 0$, smooth, spherically symmetric and compactly supported. Fix $0 < \beta < 1$ and consider $\mathscr{H}_N^{(\beta)}$ defined in (26). Let $\tilde{\varphi}_t^N$ defined in (62) with $\tilde{\varphi}_0^N = \varphi \in H^4(\mathbb{R}^3)$. Fix $\ell > 0$ and consider $k_{\ell,t}$ defined in (61). Let $\alpha = \min(\beta/2, (1-\beta)/2)$. Then there exist a unitary evolution $\mathscr{U}_{2,N}(t)$ with a quadratic (in the creation and annihilation operators) generator and constants $C, c_1, c_2 > 0$ such that*

$$\begin{aligned} \| \, e^{-it\mathscr{H}_N^{(\beta)}}W(\sqrt{N}\varphi)T(k_{\ell,0})\Omega \; - \; e^{-i\int_0^t \eta_N(s)ds} \; & W(\sqrt{N}\tilde{\varphi}_t^N)\,T(k_{\ell,t})\,\mathscr{U}_{2,N}(t)\Omega \, \|^2 \\ & \leq C\,N^{-\alpha}\,e^{c_1\exp(c_2|t|)} \end{aligned} \tag{65}$$

for all $t \in \mathbb{R}$ and N large enough.

Theorem 3 still holds if we substitute the vacuum state Ω with a sequence of states $\xi_N \in \mathscr{F}$ such that $\|\xi_N\| = 1$ and $\langle \xi_N, (\mathscr{N}^2 + \mathscr{K}^2 + \mathscr{H}_N^{(\beta)})\xi_N \rangle \le C$ uniformly in N. Here $\mathscr{K} = \int \mathrm{d}x \nabla_x a_x^* \nabla_x a_x$ is the kinetic energy operator. It is also possible to approximate the dynamics of the fluctuations by a limiting evolution $\mathscr{U}_{2,\infty}(t)$, again with a quadratic generator, but now independent of N, as shown in [7, Prop. 2.1].

While we refer to [7] for a complete proof of Theorem 3, we briefly describe here the general strategy used there. The main idea is to identify a limiting fluctuation dynamics with a quadratic generator, and then apply it to obtain the norm bound for the many body dynamics of our class of initial data. The fact that this limiting dynamics may exist is suggested by the form of the generator $\mathscr{L}_{\ell,N}(t)$ of the dynamics $\mathscr{U}_{\ell,N}$, where the cubic and quartic terms seem to vanish in the limit of large N. From (64) is apparent that, $W(f)$ and $T(k_{\ell,t})$ being unitary operators, the following proposition is sufficient to prove Theorem 3.

Proposition 1 *Let $\mathscr{U}_{\ell,N}$ defined in (64), and $\alpha = \min(\beta/2, (1-\beta)/2)$. Then, there exist a unitary quadratic evolution $\mathscr{U}_{2,N}$ and constants $C, c_1, c_2 > 0$ such that, for all $t \in \mathbb{R}$ and all N large enough,*

$$\|\mathscr{U}_{\ell,N}(t;0)\Omega - e^{-i\int_0^t \eta_N(s)ds}\mathscr{U}_{2,N}(t;0)\Omega\| \le CN^{-\alpha}\exp(\exp(c_2|t|))\,. \tag{66}$$

The proposition follows from the fact that the generator $\mathscr{L}_{\ell,N}(t)$ can be written as

$$\mathscr{L}_{\ell,N}(t) = \eta_N(t) + \mathscr{L}_{2,N}(t) + \mathscr{V}_N + \mathscr{E}_N(t)\,, \tag{67}$$

where $\eta_N(t)$ is a phase, $\mathscr{L}_{2,N}(t)$ is a quadratic generator,

$$\mathscr{V}_N = \frac{1}{2}\int \mathrm{d}x\mathrm{d}y N^{3\beta-1} V(N^\beta(x-y)) a_x^* a_y^* a_x a_y \tag{68}$$

is the interaction, and $\mathscr{E}_N(t)$ satisfies

$$|\langle \psi_1, \mathscr{E}_N(t)\psi_2\rangle| \le CN^{-\alpha}e^{K|t|}\big[\langle \psi_1, (\mathscr{K} + \mathscr{N} + 1)\psi_1\rangle + \langle \psi_2, (\mathscr{K}^2 + (\mathscr{N}+1)^2)\psi_2\rangle\big] \tag{69}$$

for all $\psi_1, \psi_2 \in \mathscr{F}$. To prove Proposition 1 we use that

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\mathscr{U}_{\ell,N}(t)\Omega - e^{-i\int_0^t \eta_N(s)\mathrm{d}s}\mathscr{U}_{2,N}(t)\Omega\|^2 = 2\mathrm{Im}\big\langle \mathscr{U}_{\ell,N}\Omega, (\mathscr{L}_{\ell,N}(t) - \mathscr{L}_{2,N}(t) - \eta_N(t))e^{-i\int_0^t \eta_N(s)\mathrm{d}s}\mathscr{U}_{2,N}(t)\Omega\big\rangle\,, \tag{70}$$

with $\mathscr{U}_{2,N}(t)$ the dynamics generated by $\mathscr{L}_{2,N}(t)$. The r.h.s. of (70) is controlled using (67) and (69):

$$\begin{aligned} |\langle \mathscr{U}_{\ell,N}(t)\Omega, (\mathscr{V}_N + \mathscr{E}_N(t))\mathscr{U}_{2,N}(t)\Omega\rangle| \\ \leq CN^{-\alpha}e^{k|t|}\Big[\langle \mathscr{U}_{\ell,N}(t)\Omega, (\mathscr{H}_N + \mathscr{N} + 1)\mathscr{U}_{\ell,N}(t)\Omega\rangle \\ + \langle \mathscr{U}_{2,N}(t)\Omega, (\mathscr{K}^2 + \mathscr{N}^2 + 1)\mathscr{U}_{2,N}(t)\Omega\rangle \Big]. \end{aligned} \tag{71}$$

The problem ends up in showing that the expectations appearing in the r.h.s. of (71) are all bounded uniformly in N. The growth of $\mathscr{N}$ and $\mathscr{H}_N$ with respect to the full dynamics $\mathscr{U}_{\ell,N}$ are controlled by means of Gronwall type estimates for the expectation of $\mathscr{N}$ and $\mathscr{L}_{\ell,N}(t)$, following the same strategy described at the end of Sect. 2 for the trace norm convergence result. The new issue here is that we also need to prove bounds for the growth of the expectation of $\mathscr{N}^2$ and $\mathscr{K}^2$ with respect to the dynamics generated by the quadratic part of the generator $\mathscr{L}_{2,N}(t)$. We prove that the quadratic generator $\mathscr{L}_{2,N}(t)$ satisfies the bounds

$$\begin{aligned} \pm(\mathscr{L}_{2,N}(t) - \mathscr{K}) &\leq Ce^{K|t|}(\mathscr{N} + 1), & (\mathscr{L}_{2,N}(t) - \mathscr{K})^2 &\leq Ce^{K|t|}(\mathscr{N} + 1)^2 \\ \pm[\mathscr{N}, \mathscr{L}_{2,N}(t)] &\leq Ce^{K|t|}(\mathscr{N} + 1), & \pm\big[\mathscr{N}^2, \mathscr{L}_{2,N}(t)\big] &\leq Ce^{K|t|}(\mathscr{N} + 1)^2 \\ \pm\dot{\mathscr{L}}_{2,N}(t) &\leq Ce^{K|t|}(\mathscr{N} + 1), & |\dot{\mathscr{L}}_{2,N}(t)|^2 &\leq Ce^{K|t|}(\mathscr{N} + 1)^2 . \end{aligned} \tag{72}$$

Using Gronwall's Lemma and the bounds in (72), we obtain

$$\begin{aligned} \langle \mathscr{U}_{2,N}(t;0)\Omega, \mathscr{N}^2\mathscr{U}_{2,N}(t;0)\Omega\rangle &\leq C\exp(c_1\exp(c_2|t|))\langle\Omega, (\mathscr{N} + 1)^2\Omega\rangle \\ \langle \mathscr{U}_{2,N}(t;0)\Omega, \mathscr{L}^2_{2,N}(t)\mathscr{U}_{2,N}(t;0)\Omega\rangle &\leq C\exp(c_1\exp(c_2|t|))\langle\Omega, (\mathscr{K} + \mathscr{N} + 1)^2\Omega\rangle . \end{aligned}$$

The last bounds, combined with the bound for $(\mathscr{L}_{2,N}(t) - \mathscr{K})^2$, also implies that

$$\langle \mathscr{U}_{2,N}(t;0)\Omega, \mathscr{K}^2\,\mathscr{U}_{2,N}(t;0)\Omega\rangle \leq C\exp(c_1\exp(c_2|t|))\langle\Omega, (\mathscr{K} + \mathscr{N} + 1)^2\Omega\rangle .$$

Note that some of the bounds in (72) would not hold if we used the correlation structure defined in (45); this is the reason why we implemented correlations through the kernel defined in (61).

Remark 3 In [7] we considered fluctuations around the non linear Schrödinger dynamics for initial states on the Fock space. For N particle initial data a more convenient approach to study fluctuations around the effective dynamics has been introduced in [26] in the mean field scaling. This approach was later exploited in [28, 29] to analyze fluctuations in the regimes up to $\beta < 1/2$. The major difficulty in the extension of these results to larger values of β is the introduction of correlations in the N particle approach proposed in [26].

4 Conclusions and Open Problems

We reported on the proof of a norm approximation for the many-body dynamics described by (26) of a particular class of initial data in the Fock space which is a good candidate to describe the ground state of trapped bosons interacting with a pair potential of the form $N^{3\beta-1}V(N^\beta x)$, with $0 < \beta < 1$. In particular we showed that for any $0 < \beta < 1$ one can approximate the fluctuation dynamics $\mathscr{U}_{\ell,N}$ defined in (64) by a quadratic evolution in norm.

Instead of considering fluctuations of the time evolution around the time dependent non linear Schrödinger equation, it is also possible to approach the problem from a static point of view. To this end, one can trap the system in a finite volume (either by imposing boundary conditions or by turning on an external potential) and one can study the difference between the many-body ground state energy and the minimum of the energy functional

$$\mathscr{E}(\varphi) = \int \mathrm{d}x\big[|\nabla\varphi(x)|^2 + (\int V)|\varphi(x)|^4\big]. \tag{73}$$

In this respect Theorem 3 suggests that a good approximation for the many-body ground state of the Hamiltonian $\mathscr{H}_N^{(\beta)}$, with $0 < \beta < 1$, may have the form $W(\sqrt{N}\varphi)S\Omega$, where φ minimizes the energy functional (73) and S is the exponential of a quadratic expression, related to the limiting quadratic evolution. Similarly, a good approximation for low-lying excited states may be of the form $W(\sqrt{N_0}\varphi)Sa^*(g_1)\dots a^*(g_k)\Omega$, for appropriate $k \in \mathbb{N}$, $N_0 = N - k$ and orbitals $g_1, \dots, g_k$ orthogonal to φ. It would be very interesting to obtain a proof of the above mentioned conjectures.

Concerning the extension of our result to the Gross-Pitaevskii regime, new ideas are needed. In fact, if we follow the same strategy that we use for $\beta < 1$, it turns out that in the Gross-Pitaevskii regime one cannot approximate the fluctuation dynamics $\mathscr{U}_{\ell,N}$ by a quadratic evolution in norm. In fact, although one can control their effect on the growth of the number of particles (needed to prove the trace norm convergence), the cubic and quartic components of the generator of $\mathscr{U}_{\ell,N}$ are not negligible in the limit of large N as soon as $\beta = 1$. In other words the fluctuation dynamics of quasi–free states is not described by a quadratic generator. One may interpret this difficulty saying that the action of $T(k_{\ell,0})$ is not sufficient to describe the correlation structure developed in the Gross-Pitaevskii regime with the precision needed to get a norm approximation result. In this perspective the analysis of the fluctuation dynamics around the Gross-Pitaevskii equation may be useful to get some information on the ground state wave function in this physically relevant regime. Vice versa some new results on the time-independent characterization of bosonic systems in the Gross-Pitaevskii regime may help the understanding of the dynamical properties of the system.

We hope to be able to address some of these problems in the next future.

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Logarithmic Sobolev Inequalities for an Ideal Bose Gas

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Abstract The aim of this work is to derive logarithmic Sobolev inequalities, with respect to the Fock vacuum state and for the second quantized Hamiltonian $d\Gamma(H^\Lambda - \mu\mathbb{I})$ of an ideal Bose gas with Dirichlet boundary conditions in a finite volume Λ, from the free energy variation with respect to a Gibbs temperature state and from the monotonicity of the relative entropy. Hypercontractivity of the semigroup $e^{-\beta d\Gamma(H^\Lambda)}$ is also deduced.

Keywords Free energy • Gibbs state • Hypercontractivity • Ideal bose gas • Logarithmic sobolev inequality • Relative entropy

1 Introduction

In the 1938 the mathematical physicist S.L. Sobolev proved the following inequality

$$\Big(\int_{\mathbb{R}^n} |\psi(x)|^p\, dx\Big)^{2/p} \leq c_n \int_{\mathbb{R}^n} |\nabla\psi(x)|^2\, dx, \qquad \psi \in C^1_c(\mathbb{R}^n)\,,$$

for $n \geq 3$, $p = \frac{2n}{n-2}$ and some constant $c_n > 0$. Due to the possible interpretation of the Dirichlet integral on the right hand side as an energy functional, their are of great use in mathematical physics and became such a basic tool of investigation in linear and nonlinear PDE, that is impossible to exaggerate their importance.

In Quantum Mechanics, Dirichlet integrals are the quadratic form of the Laplace operator $H_0 := -\Delta$ that represent the kinetic energy observable of a finite system of particles and the use of the inequality above provides, among other things, classes of possibly unbounded potentials V whose quantum Hamiltonians $H_0 + V$ are self-adjoint on the Lebesgue space $L^2(\mathbb{R}^n, dx)$.

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A. Michelangeli, G. Dell'Antonio (eds.), *Advances in Quantum Mechanics*,
Springer INdAM Series 18, DOI 10.1007/978-3-319-58904-6_7

At a more fundamental level, E. Lieb recognized in the Sobolev inequalities an *uncertainty principle* which is one of the fundamental ingredients to prove the Stability of the Matter [8].

In 1976, L. Gross [7] proved the following Logarithmic Sobolev inequality for $f \in C^1_c(\mathbb{R}^n)$ and $\|f\|_{L^2(\mathbb{R}^n,\gamma)} = 1$

$$\int_{\mathbb{R}^n} \gamma(dx)|f(x)|^2 \log|f(x)|^2 \leq \int_{\mathbb{R}^n} \gamma(dx)|\nabla f(x)|^2$$

with respect to the Gaussian probability measure $\gamma(dx) = (2\pi)^{-n/2}e^{-|x|^2/2}dx$. He demonstrated that this inequality is an infinitesimal version of the Nelson's hypercontractivity

$$\|e^{-t\widetilde{H}}u\|_{L^4(\mathbb{R}^n,\gamma)} \leq \|u\|_{L^2(\mathbb{R}^n,\gamma)}, \qquad t > 0\,, \quad u \in L^2(\mathbb{R}^n,\gamma)$$

of the Ornstein-Uhlenbeck semigroup $e^{-t\widetilde{H}}$ generated by the ground state representation $\widetilde{H}$ of the Hamiltonian $H = \frac{1}{2}(-\Delta + |x|^2 - 1)$ of the quantum harmonic oscillator (see [10]).

A first key difference between SI and LSI is that in the latter, the constant in front the Gaussian Dirichlet integral is dimension independent. This fact allowed Gross to prove LSI on infinite dimensional Gaussian Banach spaces, providing a useful tool to infinite dimensional analysis.

Both E. Nelson and L. Gross were motivated in discovering their results by the problems of constructive Quantum Field Theory where hypercontractivity and logarithmic Sobolev inequalities provide sufficient compactness near the bottom of the spectrum of free Hamiltonians H_0 to prove essential self-adjointness, lower semiboundedness, existence and finite degeneracy of the ground state as well its uniqueness in case of ergodicity, for interacting Hamiltonians $H_0 + V$ (see [6, 9] and also [13, 14]).

Among the applications of infinite dimensional LSI to Mathematical Physics, we recall the work of E. Carlen and D. Stroock [3] on the extension of the Bakry-Emery criterion and its use to prove LSI for non product Gibbs measures for continuous spin systems as well as the work of D. Stroock and B. Zegarlinski [15] about the equivalence of LSI with the Dobrushin-Shlosman mixing condition for lattice gases with compact continuous spin space.

Later, E.B. Davies and B. Simon [5] discovered that families of LSI

$$\int_X dm\,|u|^2 \log|u|^2 \leq \beta\mathscr{E}[u] + b(\beta), \qquad \beta > 0\,, \quad \|u\|_{L^2(X,\mu)} = 1$$

on a locally compact measured space (X, μ), are deeply connected with the ultracontractivity of the heat semigroup associated to the Dirichlet form $\mathscr{E}$, provided the local norm $b(\beta)$ is not too singular as β goes to zero. This theory was subsequently used by E.B. Davies [D] to get sharp off diagonal bounds upon the heat kernel of the Markovian semigroup generated by a Dirichlet form $\mathscr{E}$ satisfying such logarithmic Sobolev inequality.

The first aim of this work is prove logarithmic Sobolev inequalities LSI(Λ), with respect to the Fock vacuum state ω_F^Λ or measure μ_F^Λ, for the second quantized Hamiltonian $\beta d\Gamma(H^\Lambda - \mu\mathbb{I})$ (at fixed inverse temperature $\beta > 0$ and activity $\mu \in \mathbb{R}$) of a gas of non interacting identical particles obeying the Bose-Einstein statistics and confined in a bounded Euclidean domain where they are subject to Dirichlet boundary conditions.

Our second aim is to introduce a new approach to logarithmic Sobolev inequality based on two fundamental ideas of Quantum Statistical Mechanics, namely, the relation between *Helmholtz free energy, Gibbs states* and *relative entropy*, on one hand, and the *monotonicity of relative entropy*, on the other hand.

2 Logarithmic Sobolev Inequalities for Ideal Bosons Gas in Finite Volume

To properly state the main result of the paper and introduce notations, we start to describe the framework of the work. For the standard fundamental result we will use, we refer to the standard classical monographies [2, 13].

Warning: *Whenever a self-adjoint operator H is semi-bounded, to ease notation the expression $(\psi, H\psi)$ will be denote the value of the lower semicontinuous quadratic form of H at an element ψ of its quadratic form domain.*

Let $\Lambda \subset \mathbb{R}^d$ be a bounded Euclidean domain and H^Λ be the Dirichlet-Laplacian operator on the complex Hilbert space $\mathfrak{h}_\Lambda := L^2(\Lambda)$, considered with respect to the Lebesgue measure on Λ, defined as the closure of $-\Delta$ on the domain $C_c^\infty(\Lambda)$.

Denote by $\mathfrak{F}(\mathfrak{h}_\Lambda)$ the bosonic Fock space and by $\mathfrak{U}(h_\Lambda)$ the CCR algebra builded on $\mathfrak{h}_\Lambda$, when considered as a symplectic real vector space with the symplectic form

$$\sigma(f,g) := \operatorname{Im}(f,g)_{\mathfrak{h}_\Lambda}, \qquad f,g \in \mathfrak{h}_\Lambda .$$

The vacuum vector $\Omega \in \mathfrak{F}(h_\Lambda)$ is cyclic for $\mathfrak{U}(h_\Lambda)$ and defines on it the Fock vacuum state

$$\omega_F^\Lambda(A) := (\Omega, A\Omega)_{\mathfrak{h}_\Lambda} .$$

The annihilation and creation operators $\{a(f), a^*(f) : f \in \mathfrak{h}_\Lambda\}$ define the self-adjoint field operators $\{\Phi(f) : f \in \mathfrak{h}_\Lambda\}$

$$\Phi(f) := \overline{\frac{a(f) + a^*(f)}{\sqrt{2}}}$$

which give rise to the Weyl unitaries

$$W(f) := e^{i\Phi(f)}$$

that satisfy the Weyl's form of the Canonical Commutation Relation

$$W(f)W(g) = W(f+g)e^{-i\sigma(f,g)/2}, \qquad f, g \in \mathfrak{h}_\Lambda .$$

The subspace $L^2_{\mathbb{R}}(\Lambda)$ of real functions is a Lagrangian submanifold of $L^2(\Lambda)$ in the sense that the symplectic form vanishes identically so that the corresponding Weyl operators commute

$$W(f)W(g) = W(f+g) = W(g)W(f), \qquad f, g \in L^2_{\mathbb{R}}(\Lambda)$$

and the (double commutant) von Neumann algebra

$$\mathfrak{M}_\Lambda := \{W(f) \in \mathscr{B}(\mathfrak{F}(\mathfrak{h}_\Lambda)) : f \in L^2_{\mathbb{R}}(\Lambda)\}''$$

is abelian. By a fundamental theorem due to J. von Neumann, $\mathfrak{M}_\Lambda$ is identical with the weak closure of the subspace of linear combinations of Weyl unitaries in the algebra of all bounded operators on the Fock space.

The Fock vacuum state ω_F^Λ is normal on $\mathfrak{M}_\Lambda$ so that the pair $(\mathfrak{M}_\Lambda, \omega_F^\Lambda)$ can be realized as the abelian von Neumann algebra $L^\infty(Q_\Lambda, \mu_F^\Lambda)$ of essentially bounded measurable functions on a suitable measurable space Q_Λ, endowed with a probability measure. The fundamental relation

$$\omega_F^\Lambda(W(f)) = \omega_F^\Lambda(e^{i\Phi(f)}) = e^{-\frac{1}{4}\|f\|^2}, \qquad f \in \mathfrak{h}_\Lambda$$

allow the identification of the system of self-adjoint operators $\{\Phi(f) : f \in \mathfrak{h}_\Lambda^{\mathbb{R}}\}$ as a Gaussian random field (or process) $\{\phi(f) : f \in \mathfrak{h}_\Lambda^{\mathbb{R}}\}$ on a Gaussian space $(Q_\lambda, \mu_F^\Lambda)$, where the following relations hold true for $f, g \in \mathfrak{h}_\Lambda^{\mathbb{R}}$

$$\omega_F^\Lambda(\Phi(f)\Phi(g)) = \int_{Q_\Lambda} \phi(f)\phi(g)\, d\mu_F^\Lambda = \frac{1}{2}(f,g)_{\mathfrak{h}_\Lambda} = \frac{1}{2}\int_\Lambda f(x)g(x)dx.$$

Under the Segal isomorphism, the complex Hilbert space $L^2(Q_\Lambda, \mu_F^\Lambda)$ is identified with the Fock space $\mathfrak{F}(\mathfrak{h}_\Lambda)$ and the constant function 1 on Q_Λ is identified or with the identity $\mathbb{I}$ operator, when considered as the unit of $L^\infty(Q_\Lambda, \mu_F^\Lambda)$, or with the vacuum vector Ω, when considered as an element of $L^2(Q_\Lambda, \mu_F^\Lambda)$.

We shall make use of the particular realization of the Gaussian random process where Q_Λ is the infinite product of the one-point compactification of the real line $Q_\Lambda := \Pi_{n=1}^\infty \dot{\mathbb{R}}$ and where the Gaussian measure μ_F^Λ is the infinite product of copies of the Gaussian probability measure on $\dot{\mathbb{R}}$

$$\gamma(dx) := \pi^{-\frac{1}{2}} e^{-x^2} dx .$$

Choosing an orthonormal basis $\{f_n : n \geq 1\} \subset \mathfrak{h}_\Lambda^{\mathbb{R}}$, the field operator $\Phi(f_n)$ is identified with the multiplication operator $\phi(f_n)$ on $L^2(Q_\Lambda, \mu_F^\Lambda)$

$$(\phi(f_n)g)(x_1, \dots) = x_n g(x_1, \dots), \qquad (x_1, \dots) \in Q_\Lambda\,, \qquad g \in L^2(Q_\Lambda, \mu_F^\Lambda)\,.$$

Notice that, using the Segal isomorphism, the relative entropy $H_{\mathfrak{M}_\Lambda}(\omega_1, \omega_2)$ of restrictions to the abelian von Neumann algebra $\mathfrak{M}_\Lambda$ of states ω_1 , ω_2 of the CCR algebra $\mathfrak{U}(\mathfrak{h}_\Lambda)$, appears as

$$H_{\mathfrak{M}_\Lambda}(\omega_2, \omega_1) = \int_{Q_\Lambda} d\mu_2 \ln\Big(\frac{d\mu_2}{d\mu_1}\Big)$$

in terms of the probability measures μ_1, μ_2 on Q_Λ representing ω_1, ω_2 restricted to $\mathfrak{M}_\Lambda$, provided μ_2 is absolutely continuous with respect to μ_1.

We shall denote by

$$\omega_\beta^\Lambda(A) := \frac{\mathrm{Tr}\,(e^{-\beta K_\mu^\Lambda} A)}{\mathrm{Tr}\,(e^{-\beta K_\mu^\Lambda})} \tag{1}$$

the Gibbs grand canonical equilibrium state, at inverse temperature $\beta > 0$ and activity $\mu < \inf \sigma(H^\Lambda)$, over the CCR algebra $\mathfrak{U}(h_\Lambda)$, corresponding to the second quantization Hamiltonian $K_\mu^\Lambda := d\Gamma(H^\Lambda - \mu\mathbb{I})$ on $\mathfrak{F}(\mathfrak{h}_\Lambda)$ of the one-particle Hamiltonian $H^\Lambda - \mu\mathbb{I}$ on $L^2(\Lambda)$ [2, 5.2.5]. Concerning the existence of the Gibbs state above, notice that, since Λ is bounded then $e^{-\beta H^\Lambda}$ is trace class for any $\beta > 0$ and consequently, by [2] Proposition 5.2.27, $e^{-\beta K_\mu^\Lambda}$ is trace class too for any $\beta > 0$ (and in fact for any real μ). We shall denote by $N^\Lambda := d\Gamma(\mathbb{I})$ the number operator on $\mathfrak{F}(\mathfrak{h}_\Lambda)$. For a unit vector $\psi \in \mathfrak{F}(\mathfrak{h}_\Lambda)$, we shall denote by ω_ψ the corresponding vector state on $\mathfrak{U}(\mathfrak{h}_\Lambda)$, as well as its restriction to $\mathfrak{M}_\Lambda$.

The first step to the main result of the work is the following observation.

Lemma 1 (Free Energy Variation, Gibbs State and Relative Entropy) *Denote by N the von Neumann algebra $\mathscr{B}(\mathfrak{F}(\mathfrak{h}_\Lambda))$ of all bounded operators on the Fock space. On its normal state space $N_{*,1}$, identified with the space of nonnegative trace class operators ρ such that* $\mathrm{Tr}\,(\rho) = 1$ *(called density matrices), define the energy functional*

$$E : N_{*,1} \to [0, +\infty], \qquad E(\rho) := \mathrm{Tr}\,(\rho^{1/2} K_\mu^\Lambda \rho^{1/2}), \qquad \rho \in N_{*,1}\,,$$

the von Neumann entropy functional

$$S_N : N_{*,1} \to [0, +\infty], \qquad S_N(\rho) := -\mathrm{Tr}\,(\rho \ln \rho), \qquad \rho \in N_{*,1}\,,$$

and the Helmholtz free energy functional at inverse temperature $\beta > 0$

$$F_\beta : N_{*,1} \to [0, +\infty], \qquad F_\beta(\rho) := E(\rho) - \frac{1}{\beta} S(\rho), \qquad \rho \in N_{*,1}\,.$$

The free energy functional attains its minimum value $F_\beta(\rho_\beta) = -\beta^{-1} \ln \mathrm{Tr}\,(e^{-\beta K_\mu^\Lambda})$ *at the Gibbs state* ω_β^Λ*, represented by the density matrix* $\rho_\beta := e^{-\beta K_\mu^\Lambda} / \mathrm{Tr}\,(e^{-\beta K_\mu^\Lambda})$*. Moreover, the variation of the free energy with respect to the Gibbs state, is proportional by* β*, to the relative entropy* H_N *of the states*

$$0 \le H_N(\rho, \rho_\beta) = \beta(F(\rho) - F(\rho_\beta)), \qquad \rho \in N_{*,1}\,. \tag{2}$$

Proof We may assume that $\beta = 1$ and that $\mathrm{Tr}\,(e^{-\beta K_\mu^\Lambda}) = 1$. By the cyclicity of the trace

$$\begin{aligned} F_1(\rho_1) = E(\rho_1) - S_N(\rho_1) &= \mathrm{Tr}\,(\rho_1^{1/2} K_\mu^\Lambda \rho_1^{1/2}) + \mathrm{Tr}\,(\rho_1 \ln \rho_1) \\ &= -\mathrm{Tr}\,(\rho_1^{1/2} (\ln e^{-K_\mu^\Lambda}) \rho_1^{1/2}) + \mathrm{Tr}\,(\rho_1 \ln \rho_1) \\ &= -\mathrm{Tr}\,(\rho_1^{1/2} (\ln \rho_1) \rho_1^{1/2}) + \mathrm{Tr}\,(\rho_1 \ln \rho_1) \\ &= -\mathrm{Tr}\,(\rho_1 \ln \rho_1) + \mathrm{Tr}\,(\rho_1 \ln \rho_1) = 0 \end{aligned}$$

and, for all $\rho \in N_{*,1}$, by the definition of the relative entropy H_N (see [16]) we have

$$\begin{aligned} F_1(\rho) = E(\rho) - S_N(\rho) &= \mathrm{Tr}\,(\rho^{1/2} K_\mu^\Lambda \rho^{1/2}) + \mathrm{Tr}\,(\rho \ln \rho) \\ &= -\mathrm{Tr}\,(\rho^{1/2} (\ln \rho_1) \rho^{1/2}) + \mathrm{Tr}\,(\rho \ln \rho) \\ &= \mathrm{Tr}\,(\rho^{1/2} (\ln \rho - \ln \rho_1) \rho^{1/2}) \\ &= H_N(\rho, \rho_1)\,. \end{aligned}$$

The second step in the proof of the our main result is the following fundamental property.

Theorem 1 (Relative Entropy Monotonicity, [16] Theorem 4') *Let* $\omega_1\,, \omega_2$ *be normal states on* $N := \mathscr{B}(\mathfrak{F}(\mathfrak{h}_\Lambda))$ *and* ω_1', ω_2' *their restriction to the von Neumann subalgebra* $\mathfrak{M}_\Lambda$*. Denoting by* H_N *and* $H_{\mathfrak{M}_\Lambda}$*, the relative entropy on* N *and* $\mathfrak{M}_\Lambda$*, respectively, one has*

$$H_{\mathfrak{M}_\Lambda}(\omega_1', \omega_2') \le H_N(\omega_1, \omega_2)\,. \tag{3}$$

More explicitly, if ρ_1, ρ_2 *are the density matrices representing* ω_1, ω_2 *and* μ_1, μ_2 *are the probability measures on* Q_Λ *representing the restrictions* ω_1', ω_2', *then one has*

$$\int_{Q_\Lambda} d\mu_2 \Big(\frac{d\mu_1}{d\mu_2}\Big) \ln\Big(\frac{d\mu_1}{d\mu_2}\Big) \leq \mathrm{Tr}\,(\rho_1^{1/2}(\ln\rho_1 - \ln\rho_2)\rho_1^{1/2})\,. \tag{4}$$

The following is the main result of the work.

Theorem 2 *Let* $\Lambda \subset \mathbb{R}^d$ *be a bounded Euclidean domain and* H^Λ *be the Dirichlet-Laplacian operator on* $\mathfrak{h}_\Lambda := L^2(\Lambda)$. *Denote by* $K_\mu^\Lambda := d\Gamma(H^\Lambda - \mu\mathbb{I})$ *its second quantization on the Fock space* $\mathfrak{F}(\mathfrak{h}_\Lambda)$, *with activity* $\mu < \inf\sigma(H^\Lambda)$.

Then the following logarithmic Sobolev inequalities hold true for any $\beta > 0$ *and* $\|\psi\|_{\mathfrak{F}(\mathfrak{h}_\Lambda)} = 1$

$$H_{\mathfrak{M}_\Lambda}(\omega_\psi, \omega_F^\Lambda) \leq \beta(\psi, K_\mu^\Lambda\psi) + \ln\mathrm{Tr}\,e^{-\beta K_\mu^\Lambda} + 4d(\beta,\mu)(\psi, N^\Lambda\psi) + d(\beta,\mu) \tag{5}$$

where $z := e^{\beta\mu}$ *and* $d(\beta,\mu) := \mathrm{Tr}\,(ze^{-\beta H^\Lambda}(\mathbb{I} + ze^{-\beta H^\Lambda})^{-1})$. *In terms of the free energy of the system the inequality reads as follows*

$$H_{\mathfrak{M}_\Lambda}(\omega_\psi, \omega_F^\Lambda) \leq \beta(F(\omega_\psi) - F(\omega_\beta^\Lambda)) + 4d(\beta,\mu)(\psi, N^\Lambda\psi) + d(\beta,\mu)\,. \tag{6}$$

Notice that, when $\mathfrak{M}_\Lambda$ is identified with $L^\infty(Q_\Lambda, d\mu_F^\Lambda)$, we have

$$H_{\mathfrak{M}_\Lambda}(\omega_\psi, \omega_F^\Lambda) = \int_{Q_\Lambda} d\mu_F^\Lambda |\psi|^2 \ln|\psi|^2, \qquad \|\psi\|_{L^2(Q_\Lambda, \mu_F^\Lambda)} = 1\,.$$

Notice also that, by a classical result [4, 1.9], the following bound holds true

$$d(\beta,\mu) \leq z(1 + ze^{-\beta\lambda_0})^{-1}(4\pi\beta)^{-d/2}|\Lambda|, \qquad \beta > 0\,.$$

Proof Denoting by μ and μ_β the probability measures on Q_Λ representing the restriction to $\mathfrak{M}_\Lambda \simeq L^\infty(Q_\Lambda, \mu_F)$ of the normal states represented by the density matrix ρ and ρ_β, by Uhlmann's monotonicity theorem [16] or Theorem 1 above, we have

$$H_{\mathfrak{M}_\Lambda}(\mu, \mu_\beta) \leq H_N(\rho, \rho_\beta), \qquad \rho \in N_{*,1}$$

so that, by Lemma 1 above, the following inequality holds true

$$H_{\mathfrak{M}_\Lambda}(\mu, \mu_\beta) \leq \beta(F(\rho) - F(\rho_\beta)), \qquad \rho \in N_{*,1}\,.$$

The density matrix ρ_ψ representing a vector state ω_ψ is the orthogonal projection onto the subspace generated by ψ. On it the von Neumann entropy vanishes $S(\rho_\psi) = 0$ and the value of the energy functional is given by $E(\rho_\psi) =$

$\mathrm{Tr}\,(\rho_\psi^{1/2} K_\mu^\Lambda \rho_\psi^{1/2}) = (\psi, K_\mu^\Lambda \psi)$ so that $F(\rho_\psi) = \beta(\psi, K_\mu^\Lambda \psi)$. Denoting by $\mu_\psi = |\psi|^2 \cdot \mu_F$ the probability measure on Q_Λ representing the restriction to $\mathfrak{M}_\Lambda$ of the state represented by ρ_ψ, we obtain the following logarithmic Sobolev inequality with respect to the Gaussian measure μ_β

$$H_{\mathfrak{M}_\Lambda}(\mu_\psi, \mu_\beta) \le \beta(\psi, K_\mu^\Lambda \psi) + \ln \mathrm{Tr}\,(e^{-\beta K_\mu^\Lambda}), \qquad \|\psi\|_{\mathfrak{F}(\mathfrak{h}_\Lambda)} = 1$$

which can be written as

$$\int_{Q_\Lambda} d\mu_\psi \ln\Big(\frac{d\mu_\psi}{d\mu_\beta}\Big) \le \beta(\psi, K_\mu^\Lambda \psi) + \ln \mathrm{Tr}\,(e^{-\beta K_\mu^\Lambda}), \qquad \|\psi\|_{\mathfrak{F}(\mathfrak{h}_\Lambda)} = 1$$

and as

$$\int_{Q_\Lambda} d\mu_\beta \Big(\frac{d\mu_\psi}{d\mu_\beta}\Big) \ln\Big(\frac{d\mu_\psi}{d\mu_\beta}\Big) \le \beta(\psi, K_\mu^\Lambda \psi) + \ln \mathrm{Tr}\,(e^{-\beta K_\mu^\Lambda}), \qquad \|\psi\|_{\mathfrak{F}(\mathfrak{h}_\Lambda)} = 1\,.$$

Since

$$\frac{d\mu_\psi}{d\mu_\beta} = |\psi|^2 \frac{d\mu_F^\Lambda}{d\mu_\beta}$$

we have, for $\|\psi\|_{\mathfrak{F}(\mathfrak{h}_\Lambda)} = 1$,

$$\begin{aligned}
\int_{Q_\Lambda} d\mu_F^\Lambda \Big(\frac{d\mu_\beta}{d\mu_F^\Lambda}\Big)\Big(\frac{d\mu_\psi}{d\mu_\beta}\Big) \ln\Big(\frac{d\mu_\psi}{d\mu_\beta}\Big) &\le \beta(\psi, K_\mu^\Lambda \psi) + \ln \mathrm{Tr}\,(e^{-\beta K_\mu^\Lambda}) \\
\int_{Q_\Lambda} d\mu_F^\Lambda \Big(\frac{d\mu_\psi}{d\mu_F^\Lambda}\Big) \ln\Big(\frac{d\mu_\psi}{d\mu_\beta}\Big) &\le \beta(\psi, K_\mu^\Lambda \psi) + \ln \mathrm{Tr}\,(e^{-\beta K_\mu^\Lambda}) \\
\int_{Q_\Lambda} d\mu_F^\Lambda \Big(\frac{d\mu_\psi}{d\mu_F^\Lambda}\Big) \ln\Big(\frac{d\mu_\psi}{d\mu_F^\Lambda}\frac{d\mu_F^\Lambda}{d\mu_\beta}\Big) &\le \beta(\psi, K_\mu^\Lambda \psi) + \ln \mathrm{Tr}\,(e^{-\beta K_\mu^\Lambda}) \\
\int_{Q_\Lambda} d\mu_F^\Lambda |\psi|^2 \ln\Big(|\psi|^2 \frac{d\mu_F^\Lambda}{d\mu_\beta}\Big) &\le \beta(\psi, K_\mu^\Lambda \psi) + \ln \mathrm{Tr}\,(e^{-\beta K_\mu^\Lambda}) \\
\int_{Q_\Lambda} d\mu_F^\Lambda |\psi|^2 \ln|\psi|^2 &\le \beta(\psi, K_\mu^\Lambda \psi) + \ln \mathrm{Tr}\,(e^{-\beta K_\mu^\Lambda}) + \\
&\quad + \int_{Q_\Lambda} d\mu_F^\Lambda |\psi|^2 \ln\Big(\frac{d\mu_\beta}{d\mu_F^\Lambda}\Big)
\end{aligned} \tag{7}$$

provided we show that measure associated to the Gibbs state is absolutely continuous with respect to the one associated to the Fock vacuum state.

Since $e^{-\beta H^{\Lambda}}$ is trace class on $\mathfrak{h}_{\Lambda}$, by Proposition 5.2.7 and Theorem 5.2.8 in [2], the operator $e^{-\beta K_{\mu}^{\Lambda}}$ is trace class over the Fock space $\mathfrak{F}(\mathfrak{h}_{\Lambda})$ and the Gibbs grand canonical equilibrium state ω_{β}^{Λ} is a gauge-invariant quasi-free state over the CCR algebra $\mathfrak{U}(\mathfrak{h}_{\Lambda})$ with two-point function

$$\omega_{\beta}^{\Lambda}(a^*(f)a(g)) = (g, T_{\beta,\mu}^{\Lambda}f), \qquad f, g \in \mathfrak{h}_{\Lambda}$$

where $T_{\beta,\mu}^{\Lambda} := ze^{-\beta H^{\Lambda}}(\mathbb{I} - ze^{-\beta H^{\Lambda}})^{-1}$ and $z := e^{\beta\mu}$. Since $\omega_{F}^{\Lambda}(W(f)) = e^{-\frac{1}{4}\|f\|^2_{\mathfrak{h}_{\Lambda}}}$, by Example 5.2.18 in [2] Example 5.2.18 we have that the two-point function of the Fock vacuum state vanishes identically so that the operator T_{F}^{Λ} defined by its two-point function vanishes too

$$0 = \omega_{F}^{\Lambda}(a^*(f)a(g)) =: (g, T_{F}^{\Lambda}f), \qquad f, g \in \mathfrak{h}_{\Lambda}\,.$$

Since $T_{\beta,\mu}^{\Lambda} \leq ze^{-\beta H^{\Lambda}}(\mathbb{I} - ze^{-\beta\lambda_0})^{-1}$ then $T_{\beta,\mu}^{\Lambda}$ is a trace class operator and

$$\sqrt{T_{\beta,\mu}^{\Lambda}} - \sqrt{T_{F}^{\Lambda}} = \sqrt{T_{\beta,\mu}^{\Lambda}}$$

is an Hilbert-Schmidt operator. By [1], main Theorem p. 285, the state ω_{β}^{Λ} is quasi-equivalent to the Fock vacuum state ω_{F}^{Λ} in the sense that they have quasi-equivalent GNS representation and thus give rise to the same (abelian) von Neumann algebra $\mathfrak{M}_{\Lambda}$ which can be identified with $L^{\infty}(Q_{\Lambda}, \mu_{F}^{\Lambda})$. We thus have the mutual absolute continuity of the Gaussian measures μ_{β}^{Λ} and μ_{F}^{Λ} on Q_{Λ} representing the states ω_{β}^{Λ} and ω_{F}^{Λ}. By [12], Theorem 3, the Radon-Nikodym derivative $d\mu_{\beta}^{\Lambda}/d\mu_{F}^{\Lambda}$ is given by

$$\frac{d\mu_{\beta}^{\Lambda}}{d\mu_{F}^{\Lambda}}(f) = (\det(A))^{-1/2}\exp[(f, (\mathbb{I} - A^{-1})f)], \qquad f \in \mathfrak{h}_{\Lambda}\,,$$

where

$$A := \frac{\mathbb{I} + ze^{-\beta H^{\Lambda}}}{\mathbb{I} - ze^{-\beta H^{\Lambda}}}\,, \qquad \mathbb{I} - A^{-1} = \mathbb{I} - \frac{\mathbb{I} - ze^{-\beta H^{\Lambda}}}{\mathbb{I} + ze^{-\beta H^{\Lambda}}} = \frac{2ze^{-\beta H^{\Lambda}}}{\mathbb{I} + ze^{-\beta H^{\Lambda}}}\,,$$

provided we show that $\det A$ is well defined. In fact, since

$$0 \leq A - \mathbb{I} = \frac{2ze^{-\beta H^{\Lambda}}}{\mathbb{I} - ze^{-\beta H^{\Lambda}}} \leq \frac{2e^{\beta\mu}}{1 - e^{-\beta(\lambda_0 - \mu)}}e^{-\beta H^{\Lambda}}\,,$$

the trace class property of $e^{-\beta H^{\Lambda}}$ implies the same property for $A - \mathbb{I}$ and then

$$\det A \leq e^{\mathrm{Tr}\,(A - \mathbb{I})} < +\infty\,.$$

In particular

$$\ln \frac{d\mu_\beta^\Lambda}{d\mu_F^\Lambda}(f) = -\frac{1}{2}\ln\det A + (f, (\mathbb{I} - A^{-1})f)$$
$$= -\frac{1}{2}\ln\det A + (f, 2ze^{-\beta H^\Lambda}(\mathbb{I} + ze^{-\beta H^\Lambda})^{-1}f)\,.$$

Recall now that, in the model where the space Q_Λ of the Gaussian random process associated to $\mathfrak{h}_\Lambda$ is identified with the infinite product of the one-point compactification of the real line $Q_\Lambda := \Pi_{n=1}^\infty \dot{\mathbb{R}}$, the logarithm of the Radon-Nikodym derivative above is the random variable which associates to $(x_1, x_2, \dots) \in Q_\Lambda$ the value

$$\ln \frac{d\mu_\beta^\Lambda}{d\mu_F^\Lambda}(x_1, x_2, \dots) = -\frac{1}{2}\ln\det A + \sum_{n=1}^\infty 2ze^{-\beta\lambda_n}(1 + ze^{-\beta\lambda_n})^{-1}x_n^2\,.$$

If we choose as a basis for $\mathfrak{h}_\Lambda$ the normalized eigenfunctions $\{f_n \in \mathfrak{h}_\Lambda : n \geq 1\}$ of H^Λ corresponding to the eigenvalues $\{\lambda_n \in (0, +\infty) : n \geq 1\}$, $H^\Lambda f_n = \lambda_n f_n$, then the self-adjoint operator on the Fock space corresponding to the real random variable $\ln d\mu_\beta^\Lambda / d\mu_F^\Lambda$ is given by

$$\ln \frac{d\mu_\beta^\Lambda}{d\mu_F^\Lambda} = -\frac{1}{2}\Big(\ln\det A\Big)\mathbb{I} + \sum_{n=1}^\infty 2ze^{-\beta\lambda_n}(1 + ze^{-\beta\lambda_n})^{-1}\phi(f_n)^2\,.$$

Since by [2] Lemma 5.2.12

$$\phi(f_n)^2 \leq 2a^*(f_n)a(f_n) + \mathbb{I} = 2N(f_n) + \mathbb{I}\,,$$

we have

$$\ln \frac{d\mu_\beta^\Lambda}{d\mu_F^\Lambda} \leq -\frac{1}{2}\Big(\ln\det A\Big)\mathbb{I} + \sum_{n=1}^\infty 2ze^{-\beta\lambda_n}(1 + ze^{-\beta\lambda_n})^{-1}(2N(f_n) + \mathbb{I})\,.$$

Since moreover

$$\ln\det A = \sum_{n=1}^\infty \ln\Big(\frac{1 + ze^{-\beta\lambda_n}}{1 - ze^{-\beta\lambda_n}}\Big)\,,$$

setting

$$b(\beta,\mu) := \sum_{n=1}^{\infty} \frac{2ze^{-\beta\lambda_n}}{1+ze^{-\beta\lambda_n}} + \frac{1}{2}\ln\Big(1 - \frac{2ze^{-\beta\lambda_n}}{1+ze^{-\beta\lambda_n}}\Big),$$

$$c(\beta,\mu) := 4\sum_{n=1}^{\infty} ze^{-\beta\lambda_n}(1+ze^{-\beta\lambda_n})^{-1}$$

we have

$$\ln\frac{d\mu_\beta^\Lambda}{d\mu_F^\Lambda} \le b(\beta,\mu)\mathbb{I} + c(\beta,\mu)N\,.$$

If $d(\beta,\mu) := \sum_{n=1}^{\infty} ze^{-\beta\lambda_n}(1+ze^{-\beta\lambda_n})^{-1}$ then $b(\beta,\mu) \le d(\beta,\mu)$ and $c(\beta,\mu) = 4d(\beta,\mu)$ so that

$$\ln\frac{d\mu_\beta^\Lambda}{d\mu_F^\Lambda} \le d(\beta,\mu)\mathbb{I} + 4d(\beta,\mu)N\,. \tag{8}$$

From the *intrinsic logarithmic Sobolev inequality* (2.8) for the operator K_μ^Λ on the Gaussian space $L^2(Q_\Lambda,\mu_F^\Lambda)$ obtained above, we have

$$\int_{Q_\Lambda} d\mu_F^\Lambda\,|\psi|^2\ln|\psi|^2 \le \beta(\psi,K_\mu^\Lambda\psi) + \ln\operatorname{Tr}e^{-\beta K_\mu^\Lambda} + \int_{Q_\Lambda} d\mu_F^\Lambda\,|\psi|^2\ln\frac{d\mu_\beta^\Lambda}{d\mu_F^\Lambda} \tag{9}$$

for $\|\psi\|_{L^2(Q_\Lambda,\mu_F^\Lambda)} = 1$, which, on the Fock space, reads as follows

$$H_{\mathfrak{M}_\Lambda}(\omega_\psi,\omega_F^\Lambda) \le \beta(\psi,K_\mu^\Lambda\psi) + \ln\operatorname{Tr}e^{-\beta K_\mu^\Lambda} + (\psi,\ln\frac{d\mu_\beta^\Lambda}{d\mu_F^\Lambda}\psi) \tag{10}$$

for $\|\psi\|_{\mathfrak{F}(\mathfrak{h}_\Lambda)} = 1$. By the bound (2.8) above we have the desired logarithmic Sobolev inequalities (2.5)

$$H_{\mathfrak{M}_\Lambda}(\omega_\psi,\omega_F^\Lambda) \le \beta(\psi,K_\mu^\Lambda\psi) + \ln\operatorname{Tr}e^{-\beta K_\mu^\Lambda} + 4d(\beta,\mu)(\psi,N^\Lambda\psi) + d(\beta,\mu)$$

for $\|\psi\|_{\mathfrak{F}(\mathfrak{h}_\Lambda)} = 1$.

Corollary 1 *There exists $\beta_0 > 0$ depending on $0 < \mu < \lambda_0$ such that the following logarithmic Sobolev inequalities hold true for all $\beta \ge \beta_0$*

$$H_{\mathfrak{M}_\Lambda}(\omega_\psi,\mu_F^\Lambda) \le \beta(\psi,d\Gamma(H^\Lambda)\psi) + \ln\operatorname{Tr}e^{-\beta K_\mu^\Lambda} + z\operatorname{Tr}(e^{-\beta H^\Lambda}), \tag{11}$$

$$H_{\mathfrak{M}_\Lambda}(\omega_\psi,\mu_F^\Lambda) \le \beta(\psi,d\Gamma(H^\Lambda)\psi) + \frac{z}{1-ze^{-\beta\lambda_0}}\operatorname{Tr}(e^{-\beta H^\Lambda}) \tag{12}$$

with $\|\psi\|_{\mathfrak{F}(\mathfrak{h}_\Lambda)} = 1$.

Proof Since $K_\mu^\Lambda = d\Gamma(H^\Lambda - \mu\mathbb{I}) = d\Gamma(H^\Lambda) - \mu N$, from the theorem above we have

$$
\begin{aligned}
&H_{\mathfrak{M}_\Lambda}(\omega_\psi,\omega_F^\Lambda) \leq \\
&\qquad \leq \beta(\psi, d\Gamma(H_\Lambda)\psi) + \ln \mathrm{Tr}\, e^{-\beta K_\mu^\Lambda} + d(\beta,\mu) + (4d(\beta,\mu) - \beta\mu)(\psi, N\psi)
\end{aligned}
$$

for all $\|\psi\|_{\mathfrak{F}(\mathfrak{h}_\Lambda)} = 1$. Since $d(\beta,\mu) \leq z\mathrm{Tr}\,(e^{-\beta H^\Lambda})$ and $d(\beta,\mu)$ is decreasing to 0 as β increase to $+\infty$, there exists $\beta_0 > 0$ such that $4d(\beta,\mu) - \beta\mu \leq 0$ for all $\beta \geq \beta_0$ and we get (2.11). Finally, by Proposition 5.2.27 in [2] we have

$$
\ln \mathrm{Tr}\,(e^{-\beta K_\mu^\Lambda}) \leq z(1 - ze^{-\beta\lambda_0})^{-1}\mathrm{Tr}\,(e^{-\beta H^\Lambda})
$$

so that

$$
\begin{aligned}
\ln \mathrm{Tr}\, e^{-\beta K_\mu^\Lambda} + z\mathrm{Tr}\,(e^{-\beta H^\Lambda}) &\leq [z + z(1 - ze^{-\beta\lambda_0})^{-1}]\mathrm{Tr}\,(e^{-\beta H^\Lambda}) \leq \\
&\leq \frac{z}{1 - ze^{-\beta\lambda_0}}\mathrm{Tr}\,(e^{-\beta H^\Lambda})
\end{aligned}
$$

from which (2.12) follows.

Corollary 2 *The semigroup $\{e^{-\beta d\Gamma(H^\Lambda)} : \beta > 0\}$ is hypercontractive, i.e. it is Markovian in the sense that it is positivity preserving and contractive on $L^p(Q_\Lambda, \mu_F^\Lambda)$ for any $p \in [0, +\infty]$ and $e^{-\beta_0 H^\Lambda}$ is bounded from $L^2(Q_\Lambda, \mu_F^\Lambda)$ to $L^4(Q_\Lambda, \mu_F^\Lambda)$. In particular, the following logarithmic Sobolev inequality holds true for some $\beta_h > \beta_0$*

$$
H_{\mathfrak{M}_\Lambda}(\omega_\psi, \mu_F^\Lambda) \leq \beta_h(\psi, d\Gamma(H^\Lambda)\psi), \qquad \|\psi\|_{\mathfrak{F}(\mathfrak{h}_\Lambda)} = 1\,. \tag{13}
$$

Proof Since $\beta H^\Lambda \geq 0$ for all $\beta > 0$, then $e^{-\beta d\Gamma(H^\Lambda)} = d\Gamma(e^{-\beta H^\Lambda})$ is positive preserving (see [11]). Since, by construction, $e^{-\beta d\Gamma(H^\Lambda)}\Omega = \Omega$ for all $\beta > 0$, the semigroup is also contractive on $\mathfrak{M}_\Lambda \simeq L^\infty(Q_\Lambda, \mu_F^\Lambda)$, hence Markovian.

Fix now $0 < \mu < \lambda_0$ and consider the value β_0 determined in Corollary 2. Since, by construction, the spectrum of $d\Gamma(H^\Lambda)$ is discrete, $0 = \inf \sigma(d\Gamma(H^\Lambda))$ and the logarithmic Sobolev inequality (2.12) holds true, the stated results follow from Theorem 6.1.22 ii) in [5].

Acknowledgements This work has been supported by GREFI-GENCO INDAM Italy-CNRS France and MIUR PRIN 2012 Project No 2012TC7588-003.

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Spherical Schrödinger Hamiltonians: Spectral Analysis and Time Decay

Luca Fanelli

Abstract In this survey, we review recent results concerning the canonical dispersive flow e^{itH} led by a Schrödinger Hamiltonian H. We study, in particular, how the time decay of space L^p-norms depends on the frequency localization of the initial datum with respect to the some suitable spherical expansion. A quite complete description of the phenomenon is given in terms of the eigenvalues and eigenfunctions of the restriction of H to the unit sphere, and a comparison with some uncertainty inequality is presented.

Keywords Dispersive estimates • Electromagnetic potentials • Schrödinger equation

1 Introduction

For $\psi = \psi(t,x) : \mathbb{R} \times \mathbb{R}^d \to \mathbb{C}$, let us consider the free Schrödinger equation

$$\partial_t \psi = i\Delta\psi, \qquad \psi(0,x) = \psi_0(x). \tag{1}$$

Solving (1) with initial datum $\psi_0(x) \in L^2(\mathbb{R}^d)$ is to find a wavefunction $\psi \in \mathscr{C}^1(\mathbb{R}; L^2(\mathbb{R}^d))$ such that $\widehat{\psi}(t,\xi) = e^{-it|\xi|^2}\widehat{\psi}_0(\xi)$, the hat denoting the Fourier transform in the x-variable

$$\widehat{\psi}(t,\xi) := \int_{\mathbb{R}^d} e^{-itx\cdot\xi}\psi(t,x)\,dx.$$

Computing the distributional Fourier transform of $e^{-it|\xi|^2}$, one finds that the unique solution to (1), in the above sense, is given by

$$\psi(t,x) = (4\pi it)^{-\frac{d}{2}} e^{i\frac{|x|^2}{4t}} * \psi_0(x) = (4\pi it)^{-\frac{d}{2}} e^{i\frac{|x|^2}{4t}} \int_{\mathbb{R}^d} e^{i\frac{x\cdot y}{2t}} e^{i\frac{|y|^2}{4t}} \psi_0(y)\,dy. \tag{2}$$

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A. Michelangeli, G. Dell'Antonio (eds.), *Advances in Quantum Mechanics*,
Springer INdAM Series 18, DOI 10.1007/978-3-319-58904-6_8

From now on, we will denote by $e^{it\Delta}$ the one-parameter flow on $L^2(\mathbb{R}^d)$ defined by formula (2), namely $e^{it\Delta}\psi_0(\cdot) = \psi(t,\cdot)$, being ψ as in (2). By Plancherel Theorem it follows that $e^{it\Delta}$ is unitary on $L^2(\mathbb{R}^d)$, namely

$$\left\| e^{it\Delta}\psi_0(\cdot)\right\|_{L^2(\mathbb{R}^d)} = \|\psi_0\|_{L^2(\mathbb{R}^d)}, \qquad \forall t \in \mathbb{R}. \tag{3}$$

By (2), it also immediately follows that

$$\left\| e^{it\Delta}\psi_0(\cdot)\right\|_{L^\infty(\mathbb{R}^d)} \leqslant C|t|^{-\frac{d}{2}}\|\psi_0\|_{L^1(\mathbb{R}^d)}, \qquad \forall t \in \mathbb{R}, \tag{4}$$

with a constant $C > 0$ independent on t and ψ_0. The last inequality, together with (3), gives by Riesz-Thorin the full list of *time decay estimates* for the free Schrödinger equation

$$\left\| e^{it\Delta}\psi_0(\cdot)\right\|_{L^p(\mathbb{R}^d)} \leqslant C|t|^{-d\left(\frac{1}{2}-\frac{1}{p}\right)}\|\psi_0\|_{L^{p'}(\mathbb{R}^d)}, \qquad \forall t \in \mathbb{R}, \qquad \forall p \geqslant 2 \tag{5}$$

where the constant C only depends on p and d. Inequalities (5) turn out to be a crucial tool in Scattering Theory and Nonlinear Analysis; in particular, a suitable time average of the same leads to the so called *Strichartz estimates* (see the standard reference [23]), which play a fundamental role both for fixed point results and as Restriction Theorems for the Fourier transform:

$$\left\| e^{it\Delta}\psi_0\right\|_{L^q_tL^r_x} \leqslant C\|\psi_0\|_{L^2(\mathbb{R}^d)}, \tag{6}$$

with $2/q = d/2 - d/r$, $q \geqslant 2$ and $(q,r,d) \neq (2,\infty,2)$, and

$$\left\| e^{it\Delta}\psi_0(\cdot)\right\|_{L^p(\mathbb{R}^d)} := \left\| \left\| e^{it\Delta}\psi_0(\cdot)\right\|_{L^r(\mathbb{R}^d)}\right\|_{L^q(\mathbb{R})}.$$

From now on, we point our attention on estimate (4) and try to give it a deeper insight. First of all, it is clear by (2) that a crucial role is played by the plane wave $K(x,y) := e^{i\frac{x\cdot y}{2t}}$ which is uniformly bounded with respect to the x, y variables, for any fixed time $t \neq 0$, i.e.

$$\sup_{x,y\in\mathbb{R}^d}\left| e^{i\frac{x\cdot y}{2t}}\right| = 1 < \infty, \qquad \forall t \neq 0. \tag{7}$$

We stress that a completely analogous behavior occurs when one solves, for positive times, the Heat Equation

$$\partial_t u = \Delta u, \qquad u(0,x) = u_0(x) \in L^p(\mathbb{R}^d), \tag{8}$$

since the solution is given by the convolution

$$u(t,x) = (4\pi t)^{-\frac{d}{2}} e^{\frac{-|x|^2}{4t}} * u_0(x), \qquad (t > 0) \tag{9}$$

for all $p \in [1, +\infty]$. This shows that (8) satisfies the same a priori estimates (5) as equation (1). Notice that (1) and (8) enjoy the same scaling invariance: namely, if ψ and u solve (1) and (8), respectively, then the rescaled function ψ_λ, u_λ, where

$$f_\lambda(t,x) := f\left(\frac{t}{\lambda^2}, \frac{x}{\lambda}\right) \qquad \lambda > 0.$$

solve the same equations as ψ and u, respectively, for any $\lambda > 0$. In addition, the Gaussian decay in (9) is much smoother than the oscillating character of the fundamental solution in (2), and leads to much stronger phenomena than the ones led by the dispersive flow $e^{it\Delta}$. Nevertheless, from the point of view of estimate (4) the behavior is the same for the flows $e^{t\Delta}, e^{it\Delta}$, when $t > 0$. Our first question is the following:

A *is the time decay of the flows $e^{t\Delta}, e^{it\Delta}$ related to the lowest frequency behavior of the corresponding fundamental solutions?*

We now pass to a more precise analysis of the decay estimate in (4), to describe some additional phenomenon which is hidden in formula (2). To this aim, let us recall the *Jacobi-Anger* expansion of plane waves, which combined with the Addition Theorem for spherical harmonics (see for example [21, formula (4.8.3), p. 116] and [2, Corollary 1]) yields

$$e^{ix\cdot y} = (2\pi)^{d/2}\big(|x||y|\big)^{-\frac{d-2}{2}} \sum_{\ell=0}^{\infty} i^\ell J_{\ell+\frac{d-2}{2}}\big(|x||y|\big)\left(\sum_{m=1}^{m_\ell} Y_{\ell,m}\big(\tfrac{x}{|x|}\big)\overline{Y_{\ell,m}\big(\tfrac{y}{|y|}\big)}\right) \tag{10}$$

for all $x, y \in \mathbb{R}^d$. Here J_ν denotes the ν-th Bessel function of the first kind

$$J_\nu(t) = \left(\frac{t}{2}\right)^\nu \sum_{k=0}^{\infty} \frac{(-1)^k}{\Gamma(k+1)\Gamma(k+\nu+1)}\left(\frac{t}{2}\right)^{2k}$$

and the $Y_{\ell,m}$ are usual spherical harmonics. Recalling that $J_\nu(t) \sim t^\nu$, for $\nu \geqslant 0$, as t goes to 0, we see that an additional time-decay, for t large is hidden in formula (2), in the term $e^{i\frac{x\cdot y}{t}}$. Roughly speaking, we expect that initial data localized at higher frequencies (with respect to the spherical harmonics expansion) decay polynomially faster along a Schrödinger evolution, in suitable topologies. This leads to our second question:

B *how can the above described phenomenon be quantified, and how stable is it under lower-order perturbations?*

Looking to identity (10), the presence of spherical harmonics and special functions gives the hint that the spherical laplacian is playing an important role in the description of the above mentioned phenomena. The aim of this survey is to describe this role, giving partial answers to the above questions and leaving some open problems, corroborated by some recent results.

2 A Stationary Viewpoint: Hardy's Inequality

We devote a preliminary section to introduce an interesting stationary viewpoint of the above picture, related to some uncertainty inequalities. To this aim, we recall the well known *Hardy's inequality*:

$$\frac{(d-2)^2}{4}\int_{\mathbb{R}^d}\frac{|\psi(x)|^2}{|x|^2}\,dx \leqslant \int_{\mathbb{R}^d}|\nabla\psi(x)|^2\,dx, \qquad (d\geqslant 3) \tag{11}$$

which holds for any function $\psi \in \dot{H}^1(\mathbb{R}^d)$, being $\dot{H}^1(\mathbb{R}^d)$ the completion of $\mathscr{C}_c^\infty(\mathbb{R}^d)$ with respect to the seminorm

$$\|f\|^2_{\dot{H}^1(\mathbb{R}^d)} := \int_{\mathbb{R}^d}|\nabla f|^2\,dx,$$

taking its quotient by the equivalence relation

$$f\sim g \text{ if } \exists c\in\mathbb{R} \,:\, f=g+c.$$

The constant in front of inequality (11) is sharp, and it is not attained on any function ψ for which the right-hand side is finite, as we see in a while. Inequality (11) can be rewritten in operator terms as

$$-\Delta-\frac{\lambda}{|x|^2}\geqslant 0, \qquad \forall\lambda\leqslant\frac{(d-2)^2}{4} \qquad (d\geqslant 3). \tag{12}$$

This has to be interpreted in the sense of the associated quadratic form. The proof of (11) relies on the following fact: given a symmetric operator $\mathscr{S}$ and a skew-symmetric operator $\mathscr{A}$ on L^2, one can (formally) compute

$$0\leqslant\int_{\mathbb{R}^d}|(\mathscr{A}+\mathscr{S})\psi|^2\,dx=\int_{\mathbb{R}^d}|\mathscr{A}\psi|^2\,dx+\int_{\mathbb{R}^d}|\mathscr{S}\psi|^2\,dx-\int_{\mathbb{R}^d}\overline{\psi}\,[\mathscr{A},\mathscr{S}]\,\psi\,dx,$$

where $[\mathscr{A},\mathscr{S}]=\mathscr{A}\mathscr{S}-\mathscr{S}\mathscr{A}$. Then the choices

$$\mathscr{A}:=\nabla, \qquad \mathscr{S}:=\frac{d-2}{2}\frac{x}{|x|^2} \qquad \Rightarrow \qquad [\mathscr{A},\mathscr{S}]=\frac{(d-2)^2}{2|x|^2}$$

immediately give (11) for functions ψ smooth enough, and a regularization argument completes the proof. Also notice the equality in (11) is attained when $(\mathscr{A} + \mathscr{S})\psi \equiv 0$, which yields the maximizing function $\psi(x) = |x|^{1-\frac{d}{2}}$, and we see that $|\nabla\psi| \notin L^2$, as mentioned above. In addition, one immediately realizes that, given $\widetilde{\mathscr{A}} = \partial_r = \nabla \cdot \frac{x}{|x|}$, then

$$[\widetilde{\mathscr{A}}, \mathscr{S}] = [\mathscr{A}, \mathscr{S}] = \frac{(d-2)^2}{2|x|^2},$$

which yields the more precise inequality

$$\frac{(d-2)^2}{4}\int_{\mathbb{R}^d}\frac{|\psi(x)|^2}{|x|^2}\,dx \leqslant \int_{\mathbb{R}^d}|\partial_r\psi(x)|^2\,dx, \qquad (d \geqslant 3) \tag{13}$$

In other words, inequality (13) shows that the angular component of $-\Delta$ is not playing a role in (11)–(12). To understand this fact, it is convenient to use spherical coordinates and write

$$\Delta = \partial_r^2 + \frac{d-1}{r}\partial_r + \frac{1}{r^2}\Delta_{\mathbb{S}^{d-1}}, \tag{14}$$

being $\Delta_{\mathbb{S}^{d-1}}$ the spherical laplacian, i.e. the Laplace-Beltrami operator on the $(d-1)$-dimensional unit sphere. We recall that $-\Delta_{\mathbb{S}^{d-1}}$ is a (positive) operator with compact inverse, hence it has purely point spectrum which accumulates at infinity, which is explicitly given by the set

$$\sigma\left(-\Delta_{\mathbb{S}^{d-1}}\right) = \sigma_{\mathrm{p}}\left(-\Delta_{\mathbb{S}^{d-1}}\right) = \{\ell(\ell + d - 2)\}_{\ell=0,1,2,\dots}. \tag{15}$$

Spherical harmonics $\{Y_{\ell,m}\}$ are associated eigenfunctions, which form a complete orthonormal set in $L^2(\mathbb{S}^{d-1})$. Denoting by H_ℓ the eigenspace associated to the ℓ-th eigenvalue of $-\Delta_{\mathbb{S}^{d-1}}$, by D_ℓ its algebraic dimension, and by $H_{\ell,m}$ the space generated by $Y_{\ell,m}$, we have the well known decomposition

$$L^2(\mathbb{S}^{d-1}) = \bigoplus_{\substack{l\geqslant 0\\ 1\leqslant m\leqslant D_\ell}} H_{\ell,m}$$

Therefore any function $\psi \in L^2(\mathbb{R}^d)$ has a (unique) expansion

$$\psi(x) = \sum_{\ell=0}^{\infty}\sum_{m=1}^{D_\ell}\psi_{\ell,m}(r)Y_{\ell,m}(\omega) \qquad x = r\omega, \quad r := |x| \tag{16}$$

and moreover

$$\|f(r\omega)\|_{L^2(\mathbb{S}^{d-1})} = \sum_{\substack{\ell\geqslant 0 \\ 1\leqslant m\leqslant D_\ell}} |f_{\ell,m}|^2.$$

We can hence use (14) to write

$$\begin{aligned}\int_{\mathbb{R}^d} |\nabla\psi|^2\,dx &= -\int_{\mathbb{R}^d} \overline{\psi}\Delta\psi\,dx \\ &= \underbrace{-\int_{\mathbb{R}^d}\overline{\psi}\left(\partial_r^2\psi + \frac{d-1}{r}\partial_r\psi\right)\,dx}_{=:I} + \underbrace{\int_{\mathbb{R}^d}\frac{1}{|x|^2}\left\langle\psi, -\Delta_{\mathbb{S}^{d-1}}\psi\right\rangle_{L^2(\mathbb{S}^{d-1})}\,dx.}_{=:II}\end{aligned} \tag{17}$$

where the brackets $\langle\cdot,\cdot\rangle_{L^2(\mathbb{S}^{d-1})}$ denote the inner product in $L^2(\mathbb{S}^{d-1})$. Arguing as above we see that

$$I \geqslant \frac{(d-2)^2}{4}\int_{\mathbb{R}^d}\frac{|\psi(x)|^2}{|x|^2}\,dx, \qquad (d\geqslant 3)$$

which is inequality (13). On the other hand, it follows by (15) that

$$II \geqslant 0,$$

therefore no additional contribution to (11) is given by $-\Delta_{\mathbb{S}^{d-1}}$. Nevertheless, given $\psi\in L^2(\mathbb{R}^{d-1})$, if $\psi_{0,1}=0$ in the expansion (16) (notice that $H_{0,1}$ coincides with the space of L^2-radial functions), then by (15) it follows that

$$\langle\psi, -\Delta_{\mathbb{S}^{d-1}}\psi\rangle_{L^2(\mathbb{S}^{d-1})} \geqslant (d-1)\|\psi(\omega)\|_{L^2(\mathbb{S}^{d-1})} \qquad \text{if } \psi_{0,1}=0$$

and inequality (13) improves:

$$\int_{\mathbb{R}^d}|\partial_r\psi(x)|^2\,dx \geqslant \left(\frac{(d-2)^2}{4}+(d-1)\right)\int_{\mathbb{R}^d}\frac{|\psi(x)|^2}{|x|^2}\,dx, \quad (d\geqslant 2) \quad \psi_{0,1}=0. \tag{18}$$

Notice that the previous gives a non trivial 2D-inequality, holding on functions ψ which are orthogonal to L^2-radial functions. More in general, given $\psi\in L^2(\mathbb{R}^d)$, let

$$\ell_0 := \min\{\ell\in\mathbb{N} \text{ such that } \exists m=1,\dots,D_\ell \;:\; \psi_{\ell,m}\neq 0\}.$$

Then, by (17), the following Hardy's inequality holds:

$$\int_{\mathbb{R}^d}|\partial_r\psi(x)|^2\,dx \geqslant \left(\frac{(d-2)^2}{4}+\ell_0(\ell_0+d-2)\right)\int_{\mathbb{R}^d}\frac{|\psi(x)|^2}{|x|^2}\,dx. \qquad (d\geqslant 1) \tag{19}$$

Inequality (19) is a quantitative stationary manifestation of the phenomenon described by question **B** in the Introduction. Here it is clear that the improvement comes from the angular component of the free Hamiltonian. In addition, the above arguments clearly suggest that the sharp constant in front of inequality (19) only depends the *lowest energies*, which is reminiscent of question **A** in the Introduction.

Having this in mind, we now see how linear lower-order perturbations of the free spherical Hamiltonian can perturb the spectral picture in (15), with consequences on the Hardy's inequality (19).

Example 1 (0-Order Perturbations) For $a \in \mathbb{R}$, consider the shifted Hamiltonians in dimension $d \geqslant 3$

$$H = -\Delta + \frac{a}{|x|^2}, \qquad L = -\Delta_{\mathbb{S}^{d-1}} + a.$$

Clearly L only has point spectrum, which is just a shift of (15)

$$\sigma(L) = \sigma_{\mathrm{p}}(L) = \{\ell(\ell + d - 2) + a\}_{\ell=0,1,2,\ldots}$$

and spherical harmonics are still eigenfunctions. The corresponding Hardy's inequality is trivially

$$\left(\frac{(d-2)^2}{4} + a\right) \int_{\mathbb{R}^d} \frac{|\psi(x)|^2}{|x|^2}\, dx \leqslant \int_{\mathbb{R}^d} |\nabla \psi(x)|^2\, dx + a \int_{\mathbb{R}^d} \frac{|\psi(x)|^2}{|x|^2}\, dx. \qquad (d \geqslant 3) \tag{20}$$

More in general, if $a = a(\omega) : \mathbb{S}^{d-1} \to \mathbb{R}$, then it is still true that L as only point spectrum, but the picture is more complicated. A typical phenomenon is the formation of clusters of eigenvalues around the (shifted) free eigenvalues. The size of the clusters depends on some universal dimensional quantity related to $a(\omega)$ (see e.g. the standard references [3, 20, 29, 30, 33] and Lemma 1 below). Moreover, for the lowest eigenvalue of L we have

$$\mu_0 := \min \sigma(L) = \inf_{\omega \in \mathbb{S}^{d-1}} a(\omega).$$

One easily see by the same arguments as above that the following Hardy's inequality holds

$$\left(\frac{(d-2)^2}{4} + \mu_0\right) \int_{\mathbb{R}^d} \frac{|\psi(x)|^2}{|x|^2}\, dx \leqslant \int_{\mathbb{R}^d} \overline{\psi} H \psi\, dx. \tag{21}$$

Example 2 (1st-Order Perturbations) Let $A \in L^2_{\mathrm{loc}}(\mathbb{R}^d)$, and recall the *diamagnetic inequality*

$$|(-i\nabla + A)\psi(x)| \geqslant |\nabla|\psi(x)||.$$

This gives for free, together with (11), that

$$\frac{(d-2)^2}{4}\int_{\mathbb{R}^d}\frac{|\psi(x)|^2}{|x|^2}\,dx \leqslant \int_{\mathbb{R}^d}|(-i\nabla+A)\psi(x)|\,dx, \qquad (d\geqslant 3). \tag{22}$$

We wonder if an improvement to the best constant of inequality (22) can occur, due to the presence of an angular perturbation of the associated Hamiltonian, in the same style as in the above example. The main example we have in mind is given by the 2D-*Aharonov-Bohm* vector potential: for $\lambda\in\mathbb{R}$, consider let us denote by

$$A:\mathbb{R}^2\to\mathbb{R}^2, \qquad A(x,y):=\lambda\left(\frac{-y}{x^2+y^2},\frac{x}{x^2+y^2}\right)$$

and consider the following quadratic form

$$q[\psi]:=\int_{\mathbb{R}^2}|(-i\nabla+A)\psi|^2\,dx.$$

Since q is positive, we can consider the *Friedrichs' extension* of the self-adjoint Hamiltonian $H := -\nabla_A^2$, on the natural form domain induced by q (see Sect. 3 below for details). The angular component of H is the operator

$$L:=\left(-i\nabla_{\mathbb{S}^1}+\mathscr{A}(\omega)\right)^2, \qquad \mathscr{A}:\mathbb{S}^1\to\mathbb{S}^1, \qquad \mathscr{A}(x,y)=\lambda\left(\frac{-y}{\sqrt{x^2+y^2}},\frac{x}{\sqrt{x^2+y^2}}\right).$$

As above, L has compact inverse and its spectrum is explicitly given by

$$\sigma(L)=\sigma_{\mathrm{p}}(L)=\{(\lambda-z)^2\}_{z\in\mathbb{Z}}.$$

Therefore, the lowest eigenvalue is given by

$$\mu_0:=\min\sigma(L)=\mathrm{dist}\,(\lambda,\mathbb{Z})^2\geqslant 0$$

and we gain the following 2D-Hardy's inequality, proved in [24]

$$\mu_0\int_{\mathbb{R}^2}\frac{|\psi(x)|^2}{|x|^2}\,dx\leqslant\int_{\mathbb{R}^2}|(-i\nabla+A)\psi|^2\,dx. \tag{23}$$

As soon as $\lambda\notin\mathbb{Z}$, this is an improvement with respect to the free case $A\equiv 0$, in which such an inequality cannot hold for any function ψ such that $|\nabla\psi|\in L^2(\mathbb{R}^2)$ (since the weight $|x|^{-2}$ is not locally integrable in 2D).

In view of the above considerations, we will restrict our attention, from now on, to some scaling-critical electromagnetic Hamiltonians and we will present some recent results which partially answer to questions **A** and **B** in the Introduction of this survey.

3 Decay Estimates: Main Results

From now on, for any $x \in \mathbb{R}^d$, we denote by $x = r\omega$, $r = |x|$. Let

$$\mathbf{A} = \mathbf{A}(\omega) : \mathbb{S}^{d-1} \to \mathbb{R}^d, \qquad a = a(\omega) : \mathbb{S}^{d-1} \to \mathbb{R}$$

be 0-degree homogeneous functions, and consider the quadratic form

$$q[\psi] := \int_{\mathbb{R}^d} \left| \left(-i\nabla + \frac{A(\omega)}{r} \right) \psi(x) \right|^2 dx + \int_{\mathbb{R}^d} \frac{a(\omega)}{r^2} |\psi(x)|^2 \, dx. \tag{24}$$

As we see in the sequel, under suitable conditions, a self-adjoint Hamiltonian

$$H := \left(-i\nabla + \frac{A(\omega)}{r} \right)^2 + \frac{a(\omega)}{r^2}, \tag{25}$$

associated to q (Friedrichs' Extension) is well defined on a domain containing $L^2(\mathbb{R}^d)$, therefore the L^2-initial value problem

$$\begin{cases} i\partial_t \psi = -iH\psi, \\ \psi(0) = \psi_0 \in L^2(\mathbb{R}^d), \end{cases} \tag{26}$$

for the wavefunction $\psi = \psi(t,x) : \mathbb{R} \times \mathbb{R}^d \to \mathbb{C}$ makes sense. Here $d \geqslant 2$, and we choose a *transversal gauge* for the magnetic vector potential, i.e. we assume

$$\mathbf{A}(\omega) \cdot \omega = 0 \quad \text{for all } \omega \in \mathbb{S}^{d-1}. \tag{27}$$

Notice that equation (26) is invariant under the scaling $u_\lambda(x,t) := u(x/\lambda, t/\lambda^2)$, which is the same of the free Schrödinger equation.

The aim is to understand the role of the spherical operator L associated to H, defined by

$$L = \big(-i\, \nabla_{\mathbb{S}^{d-1}} + \mathbf{A} \big)^2 + a(\omega), \tag{28}$$

where $\nabla_{\mathbb{S}^{d-1}}$ is the spherical gradient on the unit sphere $\mathbb{S}^{d-1}$. Assuming $a \in L^\infty(\mathbb{S}^{d-1};\mathbb{R}), \mathbf{A} \in \mathscr{C}^1(\mathbb{S}^{d-1};\mathbb{R}^d)$, then the spectrum of the operator L is formed by a diverging sequence of real eigenvalues with finite multiplicity $\mu_0(\mathbf{A},a) \leqslant \mu_1(\mathbf{A},a) \leqslant \cdots \leqslant \mu_k(\mathbf{A},a) \leqslant \cdots$ (see e.g. [16, Lemma A.5]), where each eigenvalue is repeated according to its multiplicity. Moreover we have that $\lim_{k\to\infty} \mu_k(\mathbf{A},a) = +\infty$. To each $k \geqslant 1$, we can associate a $L^2\big(\mathbb{S}^{d-1},\mathbb{C}\big)$-normalized eigenfunction φ_k of the operator L on $\mathbb{S}^{d-1}$ corresponding to the k-th eigenvalue $\mu_k(\mathbf{A}, a)$, i.e. satisfying

$$\begin{cases} L\varphi_k = \mu_k(\mathbf{A}, a)\,\varphi_k, & \text{in } \mathbb{S}^{d-1}, \\ \int_{\mathbb{S}^{d-1}} |\varphi_k|^2 \, dS(\theta) = 1. \end{cases} \tag{29}$$

In particular, if $d = 2$, φ_k are one-variable 2π-periodic functions, i.e. $\varphi_k(0) = \varphi_k(2\pi)$. Since the eigenvalues $\mu_k(\mathbf{A}, a)$ are repeated according to their multiplicity, exactly one eigenfunction φ_k corresponds to each index $k \geqslant 1$. We can choose the functions φ_k in such a way that they form an orthonormal basis of $L^2(\mathbb{S}^{d-1}, \mathbb{C})$. We also introduce the numbers

$$\alpha_k := \frac{d-2}{2} - \sqrt{\left(\frac{d-2}{2}\right)^2 + \mu_k(\mathbf{A}, a)}, \quad \beta_k := \sqrt{\left(\frac{d-2}{2}\right)^2 + \mu_k(\mathbf{A}, a)}, \tag{30}$$

so that $\beta_k = \frac{d-2}{2} - \alpha_k$, for $k = 1, 2, \ldots$.

Under the condition

$$\mu_0(\mathbf{A}, a) > -\frac{(d-2)^2}{4} \tag{31}$$

the quadratic form q in (24) associated to H is positive definite, and the Friedrichs' extension of H is well defined, with domain

$$\mathscr{D} := \left\{ f \in H^1_*(\mathbb{R}^d) : \; Hf \in L^2(\mathbb{R}^d) \right\}, \tag{32}$$

where $H^1_*(\mathbb{R}^d)$ is the completion of $C^\infty_c(\mathbb{R}^d \setminus \{0\}, \mathbb{C})$ with respect to the norm

$$\|f\|_{H^1_*(\mathbb{R}^d)} = \left(\int_{\mathbb{R}^N} \left(|\nabla f(x)|^2 + \frac{|f(x)|^2}{|x|^2} + |f(x)|^2 \right) dx \right)^{1/2}.$$

By the Hardy's inequality (11), $H^1_*(\mathbb{R}^d) = H^1(\mathbb{R}^d)$ with equivalent norms if $d \geqslant 3$, while $H^1_*(\mathbb{R}^d)$ is strictly smaller than $H^1(\mathbb{R}^d)$ if $d = 2$. Furthermore, from condition (31) and [16, Lemma 2.2], it follows that $H^1_*(\mathbb{R}^d)$ coincides with the space obtained by completion of $C^\infty_c(\mathbb{R}^d \setminus \{0\}, \mathbb{C})$ with respect to the norm naturally associated to H, i.e.

$$q[\psi] + \|\psi\|_2^2.$$

We remark that H could be not essentially self-adjoint. Indeed, in the case $\mathbf{A} \equiv 0$, Kalf, Schmincke, Walter, and Wüst [22] and Simon [28] proved that H is essentially self-adjoint if and only if $\mu_0(\mathbf{0}, a) \geqslant -\left(\frac{d-2}{2}\right)^2 + 1$ and, consequently, admits a unique self-adjoint extension (which coincides with the Friedrichs' extension); otherwise, i.e. if $\mu_0(\mathbf{0}, a) < -\left(\frac{d-2}{2}\right)^2 + 1$, H is not essentially self-adjoint and admits infinitely many self-adjoint extensions, among which the Friedrichs' extension is the only one whose domain is included in the domain of the associated quadratic form (see also [9, Remark 2.5]).

The Friedrichs' extension H naturally extends to a self adjoint operator on the dual $\mathscr{D}^\star$ of $\mathscr{D}$ and the unitary group e^{-itH} extends to a group of isometries on the dual of $\mathscr{D}$ which will be still denoted as e^{-itH} (see [6], Section 1.6 for further details). Then for every $\psi_0 \in L^2(\mathbb{R}^d)$,

$$\psi(t,x) := e^{-itH}\psi_0(x) \in \mathscr{C}(\mathbb{R}; L^2(\mathbb{R}^d)) \cap \mathscr{C}^1(\mathbb{R}; \mathscr{D}^\star),$$

is the unique solution to (26).

Now, by means of (29) and (30) define the following kernel:

$$K(x,y) = \sum_{k=-\infty}^{\infty} i^{-\beta_k} j_{-\alpha_k}(|x||y|)\varphi_k\left(\tfrac{x}{|x|}\right)\overline{\varphi_k\left(\tfrac{y}{|y|}\right)}, \tag{33}$$

where

$$j_\nu(r) := r^{-\frac{d-2}{2}} J_{\nu+\frac{d-2}{2}}(r)$$

and J_ν denotes the usual Bessel function of the first kind

$$J_\nu(t) = \left(\frac{t}{2}\right)^\nu \sum_{k=0}^{\infty} \frac{(-1)^k}{\Gamma(k+1)\Gamma(k+\nu+1)}\left(\frac{t}{2}\right)^{2k}.$$

Notice that (33) reduces to (10), in the free case $\mathbf{A} \equiv a \equiv 0$. The first result we mention in this survey is the following representation formula for e^{-itH}:

Theorem 1 (L. Fanelli, V. Felli, M. Fontelos, A. Primo—[12]) *Let $d \geqslant 3$, $a \in L^\infty(\mathbb{S}^{d-1}, \mathbb{R})$ and $\mathbf{A} \in C^1(\mathbb{S}^{d-1}, \mathbb{R}^N)$, and assume (27) and (31). Then, for any $\psi_0 \in L^2(\mathbb{R}^d)$,*

$$e^{-itH}\psi_0(x) = \frac{e^{\frac{i|x|^2}{4t}}}{i(2t)^{d/2}} \int_{\mathbb{R}^d} K\left(\frac{x}{\sqrt{2t}}, \frac{y}{\sqrt{2t}}\right) e^{i\frac{|y|^2}{4t}} \psi_0(y)\, dy. \tag{34}$$

As an immediate consequence, we see by (34) that the analog to condition (7) gives for H the complete list of usual time decay estimates (5):

Corollary 1 *Let $d \geqslant 3$, $a \in L^\infty(\mathbb{S}^{d-1}, \mathbb{R})$ and $\mathbf{A} \in C^1(\mathbb{S}^{d-1}, \mathbb{R}^N)$, and assume (27) and (31). If*

$$\sup_{x,y\in\mathbb{R}^d} |K(x,y)| < \infty, \tag{35}$$

then

$$\left\|e^{-itH}\psi_0(\cdot)\right\|_{L^p(\mathbb{R}^d)} \leqslant C|t|^{-d\left(\frac{1}{2}-\frac{1}{p}\right)}\|\psi_0\|_{L^{p'}(\mathbb{R}^d)}, \qquad \forall t \in \mathbb{R}, \qquad \forall p \geqslant 2, \tag{36}$$

for some $C > 0$ *independent on* ψ_0.

In the two last decades, estimates (36) were intensively studied by several authors. The following is an incomplete list of results about this topic [1, 7, 8, 10, 11, 17, 18, 25–27, 31, 32, 34–37]. In all these papers, the potentials are sub-critical with respect to the functional scale of the Hardy's inequality (11): in other words, the critical potentials in (25) are never considered, and it does not seem that one could handle them by perturbation techniques, which are a common factor of all the above mentioned papers. Now, formula (34) and Corollary 1 give a usual tool to reduce matters to prove time decay, to a spectral analysis problem. This allowed us to prove some new positive results concerning with estimates (36). In 2D, the picture is quite well understood, thanks to the following theorem.

Theorem 2 (L. Fanelli, V. Felli, M. Fontelos, A. Primo—[13]) *Let* $d = 2$*,* $a \in W^{1,\infty}(\mathbb{S}^1, \mathbb{R})$*,* $\mathbf{A} \in W^{1,\infty}(\mathbb{S}^1, \mathbb{R}^2)$ *satisfying* (27) *and* $\mu_1(\mathbf{A}, a) > 0$*, and* H *be given by* (25)*. Then, for any* $\psi_0 \in L^2(\mathbb{R}^d) \cap L^{p'}(\mathbb{R}^d)$*,*

$$\left\|e^{-itH}\psi_0(\cdot)\right\|_{L^p(\mathbb{R}^2)} \leqslant C|t|^{-2\left(\frac{1}{2}-\frac{1}{p}\right)}\|\psi_0\|_{L^{p'}(\mathbb{R}^2)}, \qquad \forall t \in \mathbb{R}, \qquad \forall p \geqslant 2, \tag{37}$$

for some $C > 0$ *independent on* ψ_0.

Theorem 2 is proved in [13]. The core consists in proving that (35) holds, and a crucial role is played by the following Lemma, which gives a quite explicit expansion of eigenvalues and eigenfunctions of L, generalizing the results in [20]:

Lemma 1 (L. Fanelli, V. Felli, M. Fontelos, A. Primo—[13]) *Let* $a \in W^{1,\infty}(\mathbb{S}^1)$*,* $\widetilde{a} := \frac{1}{2\pi}\int_0^{2\pi} a(s)\,ds$*,* $\mathbf{A} \in W^{1,\infty}(\mathbb{S}^1)$ *such that*

$$\widetilde{\mathbf{A}} = \frac{1}{2\pi}\int_0^{2\pi} A(s)\,ds \notin \frac{1}{2}\mathbb{Z}. \tag{38}$$

Then there exist $k^*, \ell \in \mathbb{N}$ *such that* $\{\mu_k : k > k^*\} = \{\lambda_j : j \in \mathbb{Z}, |j| \geqslant \ell\}$*,*

$$\sqrt{\lambda_j - \widetilde{a}} = (\operatorname{sgn} j)\Big(\widetilde{\mathbf{A}} - \big\lfloor \widetilde{\mathbf{A}} + \tfrac{1}{2}\big\rfloor\Big) + |j| + O\big(\tfrac{1}{|j|^3}\big), \quad \text{as } |j| \to +\infty$$

and

$$\lambda_j = \widetilde{a} + \Big(j + \widetilde{\mathbf{A}} - \big\lfloor \widetilde{\mathbf{A}} + \tfrac{1}{2}\big\rfloor\Big)^2 + O\big(\tfrac{1}{j^2}\big), \quad \text{as } |j| \to +\infty. \tag{39}$$

Furthermore, for all $j \in \mathbb{Z}$, $|j| \geqslant \ell$, there exists a $L^2\big(\mathbb{S}^1, \mathbb{C}\big)$-normalized eigenfunction φ_j of the operator L on $\mathbb{S}^1$ corresponding to the eigenvalue λ_j such that

$$\varphi_j(\theta) = \frac{1}{\sqrt{2\pi}} e^{-i\left(\lfloor\widetilde{\mathbf{A}}+1/2\rfloor\theta + \int_0^\theta A(t)\,dt\right)} \left(e^{i(\widetilde{\mathbf{A}}+j)\theta} + R_j(\theta)\right), \tag{40}$$

where $\|R_j\|_{L^\infty(\mathbb{S}^1)} = O\big(\frac{1}{|j|^3}\big)$ as $|j| \to \infty$. In the above formula $\lfloor\cdot\rfloor$ denotes the floor function $\lfloor x\rfloor = \max\{k \in \mathbb{Z} : k \leqslant x\}$.

Analogous results to Lemma 1 can be proved (and are in part available) in higher dimension $d \geqslant 3$. Nevertheless, the higher dimensional scenario is quite more complicate, and some chaotic behavior of the eigenvalues of L can occur. This makes the generic validity of (36) completely unclear in dimension $d \geqslant 3$. In this direction, the only result which is available at the moment is concerned with the 3D-inverse square electric potential, and reads as follows:

Theorem 3 (L. Fanelli, V. Felli, M. Fontelos, A. Primo—[12]) *Let $d = 3$, $\mathbf{A} \equiv 0$ and $a(\omega) \equiv a \in \mathbb{R}$, with $a > -\frac{1}{4}$.*

i) If $a \geqslant 0$, then, for any $\psi_0 \in L^2(\mathbb{R}^3) \cap L^{p'}(\mathbb{R}^3)$,

$$\left\|e^{-itH}\psi_0(\cdot)\right\|_{L^p(\mathbb{R}^2)} \leqslant C|t|^{-3\left(\frac{1}{2}-\frac{1}{p}\right)} \|\psi_0\|_{L^{p'}(\mathbb{R}^2)}, \qquad \forall t \in \mathbb{R}, \qquad \forall p \geqslant 2, \tag{41}$$

for some $C > 0$ which does not depend on ψ_0.

ii) If $-\frac{1}{4} < a < 0$, let α_1 as in (30), and define

$$\|\psi\|_{p,\alpha_1} := \left(\int_{\mathbb{R}^3} (1 + |x|^{-\alpha_1})^{2-p} |\psi(x)|^p \, dx\right)^{1/p}, \quad p \geqslant 1.$$

Then the following estimates hold

$$\left\|e^{-itH}\psi_0(\cdot)\right\|_{p,\alpha_1} \leqslant \frac{C(1 + |t|^{\alpha_0})^{1-\frac{2}{p}}}{|t|^{3\left(\frac{1}{2}-\frac{1}{p}\right)}} \|\psi\|_{p',\alpha_0}, \quad p \geqslant 2, \quad \frac{1}{p} + \frac{1}{p'} = 1, \tag{42}$$

for some constant $C > 0$ which does not depend on ψ_0.

Remark 1 It is interesting to remark that, in the range $-1/4 < a < 0$, (41) does not hold, while the full set of usual Strichartz estimates hold (see [4, 5]). This is now clearly understood in terms of formula (34): notice that, if $a = \mu_0 < 0$, then $\alpha_0 > 0$ and a negative-index Bessel function appears in the kernel K given by (33); since negative-index functions J_ν are singular at the origin, one cannot either expect the solution (34) to be in L^∞.

This can be proved as a general fact:

Theorem 4 (L. Fanelli, V. Felli, M. Fontelos, A. Primo—[13]) *Let $d \geqslant 3$, $a \in L^\infty(\mathbb{S}^{d-1}, \mathbb{R})$, $\mathbf{A} \in C^1(\mathbb{S}^{d-1}, \mathbb{R}^d)$, and assume (27), (31), and $\mu_0 < 0$. Then, for almost every $t \in \mathbb{R}$, $e^{-itH}(L^1) \nsubseteq L^\infty$; in particular e^{-itH} is not a bounded operator from $L^1(\mathbb{R}^d)$ to $L^\infty(\mathbb{R}^d)$.*

The above phenomenon can be quantified. To this aim, let us restrict our attention to the case

$$H = -\Delta + \frac{a}{|x|^2}, \qquad x \in \mathbb{R}^3.$$

Let us define

$$V_{n,j}(x) = |x|^{-\alpha_j} e^{-\frac{|x|^2}{4}} P_{j,n}\Big(\frac{|x|^2}{2}\Big)\psi_j\Big(\frac{x}{|x|}\Big), \quad n, j \in \mathbb{N},\ j \geqslant 1, \tag{43}$$

where $P_{j,n}$ is the polynomial of degree n given by

$$P_{j,n}(t) = \sum_{i=0}^{n} \frac{(-n)_i}{\big(\frac{d}{2} - \alpha_j\big)_i} \frac{t^i}{i!},$$

denoting as $(s)_i$, for all $s \in \mathbb{R}$, the Pochhammer's symbol

$$(s)_i = \prod_{j=0}^{i-1}(s+j), \qquad (s)_0 = 1.$$

Moreover, for all $k > 1$, define

$$\mathscr{U}_k = \operatorname{span}\big\{V_{n,j} : n \in \mathbb{N}, 1 \leqslant j < k\big\} \subset L^2(\mathbb{R}^N).$$

The functions $V_{n,j}$ spans $L^2(\mathbb{R}^3)$ (see [14] for details). Moreover, as initial data for (1), these functions have a quite explicit evolution: indeed, denoting by $\widetilde{V}_{n,j} := V_{n,j}/\|V_{n,j}\|_2$, the following identity holds:

$$\begin{aligned} e^{-itH}\widetilde{V}_{n,j}(x) &= e^{it\left(-\Delta + \frac{a}{|x|^2}\right)} V_{n,j}(x) \qquad (44)\\ &= (1+t^2)^{-\frac{d}{4}+\frac{\alpha_j}{2}} |x|^{-\alpha_j} \frac{e^{\frac{-|x|^2}{4(1+t^2)}}}{\|V_{n,j}\|_{L^2(\mathbb{R}^d)}} e^{i\frac{|x|^2 t}{4(1+t^2)}} e^{-i\gamma_{n,j}\arctan t} \psi_j\big(\tfrac{x}{|x|}\big) P_{n,j}\big(\tfrac{|x|^2}{2(1+t^2)}\big). \end{aligned}$$

Formula (44) has been proved in [14]. Clearly, if $a = \mu_0 \geqslant 0$, then $\alpha_0 \leqslant 0$ and the first function $\widetilde{V}_{1,0}$ decays polynomially faster than usual, in a weighted space. This is reminiscent to question **B** in the Introduction, and gives us the following evolution version of the frequency-dependent Hardy's inequality (19):

Theorem 5 (L. Fanelli, V. Felli, M. Fontelos, A. Primo—[14]) *Let $d = 3$, $a = \mu_0 \geqslant 0$, α_0 as in (30).*

(i) There exists $C > 0$ such that, for all $\psi_0 \in L^2(\mathbb{R}^3)$ with $|x|^{-\alpha_0}\psi_0 \in L^1(\mathbb{R}^3)$,

$$\left\| |x|^{\alpha_0} e^{-itH}\psi_0(\cdot) \right\|_{L^\infty} \leqslant C|t|^{-\frac{3}{2}+\alpha_0} \| |x|^{-\alpha_0}\psi_0 \|_{L^1}.$$

(ii) For all $k \in \mathbb{N}$, $k \geqslant 1$, there exists $C_k > 0$ such that, for all $\psi_0 \in \mathscr{U}_k^{\perp}$ with $|x|^{-\alpha_k}\psi_0 \in L^1(\mathbb{R}^3)$,

$$\left\| |x|^{\alpha_k} e^{-itH}\psi_0(\cdot) \right\|_{L^\infty} \leqslant C_k|t|^{-\frac{3}{2}+\alpha_k} \| |x|^{-\alpha_k}\psi_0 \|_{L^1}.$$

Some analogous results, only concerning with the decay of the first frequency space, had been previously proven in [15, 19].

To complete the survey, we leave some open questions.

(i) Concerning Theorems 2, 3, does any general result hold in dimension $d \geqslant 3$?
(ii) In what extent can one perturb the models in (25)? What is the real role played by the scaling invariance?
(iii) The proof of formula (34) strongly relies on some pseudoconformal law associated to the free Schrödinger flow (Appell transform; see [12]). Is there any analog for other dispersive models, e.g. the wave equation?
(iv) One can use formula (34) to represent the wave operators

$$W_{\pm} := L^2 - \lim_{t\to\pm\infty} e^{itH}e^{-itH_0}, \qquad H_0 := -\Delta.$$

What can one prove about the boundedness of $W_{\pm}$ in $L^p(\mathbb{R}^d)$, in the same style as in [31, 32, 34–37] (at least in 2D, having in mind Theorem 2.
(v) By standard $TT^{\star}$-arguments, one can obtain some weighted Strichartz estimates by Theorem 5. Which kind of informations do these estimates give for nonlinear Schrödinger equations associated to H?

Acknowledgements The author sincerely thanks all the organizers of the event *Contemporary Trends in the Mathematics of Quantum Mechanics* for the kind invitation, in particular Alessandro Michelangeli for his job. A special acknowledgement is to Prof. Gianfausto Dell'Antonio, for his beautiful scientific contributions, for his teachings, and for his friendship.

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On the Ground State for the NLS Equation on a General Graph

Domenico Finco

Abstract We review some recent results on the existence of the ground state for a nonlinear Schrödinger equation (NLS) posed on a graph or network composed of a generic compact part to which a finite number of half-lines are attached. In particular we concentrate on the main theorem in Cacciapuoti et al. (Ground state and orbital stability for the NLS equation on a general starlike graph with potentials, preprint arXiv:1608.01506) which covers the most general setting and we compare it with similar results.

Keywords Concentration-compactness techniques • Quantum graphs • Nonlinear Schrödinger equation

1 Introduction

Analysis on metric graphs and networks is a growing subject with many potential applications of physical and technological character. The interest in these structures, also from a mathematical point of view lies in the fact that they are relatively simple analytically, being essentially one dimensional, but on the other hand they can have in a sense arbitrary complexity due to nontrivial connectivity and topology.

A large part of the literature is devoted to linear equations on graphs (see [15, 30] for an overview of theory and the many applications), as limit model for propagation of waves in thin domains where the transverse dimensions are much smaller than the longitudinal one. A special emphasis is placed on Schrödinger equation describing the so called quantum graphs. Recently nonlinear equations have attracted attention, and a certain amount of mathematical work has been done on nonlinear Schrödinger equation on quantum graphs, at least in some special situations. The NLS is used in many situations, among them we mention the propagations of pulses in nonlinear Kerr media and the dynamics of Bose-Einstein condensates. A relevant feature of NLS in homogeneous media, or in general in presence of symmetries, is that it

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A. Michelangeli, G. Dell'Antonio (eds.), *Advances in Quantum Mechanics*, Springer INdAM Series 18, DOI 10.1007/978-3-319-58904-6_9

admits solitons or traveling waves, non dispersive solutions which evolves rigidly translating without modifying their profile. The NLS on graphs can be used as model for a number of phenomena: propagation and splitting of pulses in various optical devices such as Y-junctions, H-junctions and others, symmetry breaking due to defects and formation of pinned stationary states around the inhomogeneities, (see for example [2–4, 6, 8, 11–14, 17, 27, 29, 32, 33]; a review with references to related physical research is in [31]). Such pinned states may have relevant influence on the dynamics of traveling waves producing effective potentials well and capturing part of incoming waves. The mathematical analysis of such situation is very difficult with very few rigorous results, see [35, 36].

A first relevant question has been recently addressed in a wide generality at mathematical level is the existence of the ground state for the focusing NLS with power nonlinearity on a graph. That is the existence of an absolute minimizer of the energy functional with a mass constraint. Here we review the main theorem in [18] which provides the most general setting. In Sect. 2 we give a precise statement of the theorem and give some ideas of proof while in Sect. 3 we discuss some other recent related results in the literature.

2 Main Result

In this section we present and discuss the main theorem in [18]. We skip technical details and omit proofs referring to the original paper.

We consider a connected metric graph $\mathscr{G} = (V, E)$ where V is the set of vertices and E is the set of edges. We assume that the cardinalities $|V|$ and $|E|$ of V and E are finite. We identify each edge $e \in E$ with length $L_e \in (0, \infty]$ with the interval $I_e = [0, L_e]$, if L_e is finite, or $[0, \infty)$, if L_e is infinite. The set of edges with finite length is denoted by E^{in} while the set of edges with infinite length is denoted by E^{ex}. Moreover we associate each finite length edge with two vertices, and each infinite length edges with one vertex. The notation $\underline{v} \in e$ with $\underline{v} \in V$ and $e \in E$, denotes that $\underline{v}$ is a vertex of the edge e. Two vertices $\underline{v}_1$ and $\underline{v}_2$ are adjacent, $\underline{v}_1 \sim \underline{v}_2$ if they are vertices of a common edge which connects them. The degree of a vertex is the number of edges emanating from it. We denote by $\{e \prec \underline{v}\}$ the set of edges connecting the vertex e. We fix a coordinate x on each interval I_e such that $x = 0$ and $x = L_e$ correspond to vertices if $L_e < \infty$ while if $L_e = \infty$ the vertex attached to the rest of the graph corresponds to $x = 0$. Any choice of orientation of finite length edges is equivalent for our purposes. To avoid ambiguities, from now on we will denote points on the graph with $\underline{x} = (e, x)$, where $e \in E$ identifies the edge and $x \in I_e$ is the coordinate on the corresponding edge. In this paper we will assume that there is at least one edge with infinite length, so that the considered graph is non compact. A function $\Psi : \mathscr{G} \to \mathbb{C}$ is equivalent to a family of functions $\{\psi_e\}_{e\in E}$ with $\psi_e : I_e \to \mathbb{C}$. In our notation, if $\underline{x} = (e, x)$

$$\Psi(\underline{x}) = \psi_e(x).$$

The spaces $L^p(\mathscr{G})$, $1 \leqslant p \leqslant \infty$, are made of functions Ψ such that $\psi_e \in L^p(I_e)$ for all $e \in E$ and

$$\|\Psi\|_p^p = \sum_{e\in E} \|\psi_e\|_{L^p(I_e)}^p, \; 1 \leqslant p < \infty \qquad \|\Psi\|_\infty = \max_{e\in E} \|\psi_e\|_{L^\infty(I_e)}.$$

We denote by $(\cdot, \cdot)$ the inner product associated with $L^2(\mathscr{G})$. When $p = 2$, the index will be omitted We denote by $C(\mathscr{G})$ the set of continuous functions on $\mathscr{G}$ and introduce the spaces

$$H^1(\mathscr{G}) := \left\{\Psi \in C(\mathscr{G}) \text{ s.t. } \psi_e \in H^1(I_e) \; \forall e \in E\right\}$$

equipped with the norm

$$\|\Psi\|_{H^1(\mathscr{G})}^2 = \sum_{e\in E} \|\psi_e\|_{H^1(I_e)}^2.$$

and

$$H^2(\mathscr{G}) := \left\{\Psi \in H^1(\mathscr{G}) \text{ s.t. } \psi_e \in H^2(I_e) \; \forall e \in E\right\}$$

equipped with the norm

$$\|\Psi\|_{H^2(\mathscr{G})}^2 = \sum_{e\in E} \|\psi_e\|_{H^2(I_e)}^2.$$

In the following, whenever a functional norm refers to a function defined on the graph, we omit the symbol $\mathscr{G}$.

Here we consider a connected graph $\mathscr{G}$, composed by a compact core to which a finite number of half-lines are attached (and at least one), see Fig. 1, and a defocusing NLS with power nonlinearity of the form

$$i\frac{d}{dt}\Psi = H\Psi - |\Psi|^{2\mu}\Psi. \tag{1}$$

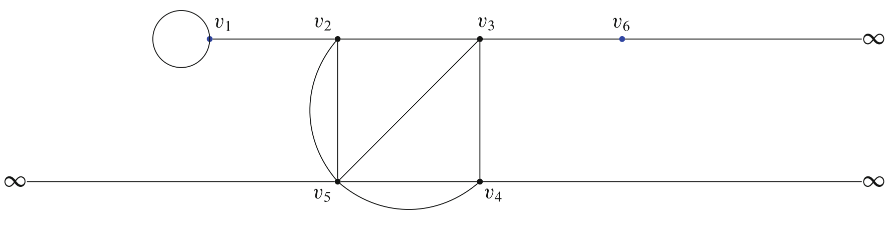

Fig. 1 13 edges (10 interior, 3 exterior); 6 vertices

We denote by H the Hamiltonian with a δ-coupling of strength $\alpha(\underline{v}) \in \mathbb{R}$ at each vertex and a potential term W on each edge. It is defined as the operator in $L^2(\mathscr{G})$ with domain

$$\mathscr{D}(H) := \left\{ \Psi \in H^2 \text{ s.t. } \sum_{e \prec \underline{v}} \partial_o \psi_e(\underline{v}) = \alpha(\underline{v})\psi_e(\underline{v}) \quad \forall \underline{v} \in V \right\}.$$

where we have denoted by ∂_o the outward derivative from the vertex, it coincides with $\frac{d}{dx}$ or $-\frac{d}{dx}$ according to the orientation on the edge. The action of H is defined by

$$(H\Psi)_e = -\psi_e'' + W_e \psi_e,$$

where W_e is the component of the potential W on the edge e. If one has in mind as reference physical model, the propagation of concentrated wave packets, the compact core plays the role of a quantum logic port that is, it reflects, splits and transmits the pulses into the infinite edges as a sort of black box scattering. The complexity of the graph together with a δ-interaction in should cover a large class of possibilities. This phenomenon was discussed at the linear level in [21] in the free case ($W = 0$), where it was proved that for a graph made by N half lines and one vertex, all the time reversal conditions can be approximated by suitable rescaled compact core with δ interactions in the added vertices.

We make very weak hypothesis in the potential W:

Assumption 1 *$W = W_+ - W_-$ with $W_\pm \geqslant 0$, $W_+ \in L^1(\mathscr{G}) + L^\infty(\mathscr{G})$, and $W_- \in L^r(\mathscr{G})$ for some $r \in [1, 1 + 1/\mu]$.*

The quadratic form of this operator is defined on the energy space given by $H^1(\mathscr{G})$ and it is explicitly given by

$$E^{lin}[\Psi] = \|\Psi'\|^2 + (\Psi, W\Psi) + \sum_{\underline{v} \in V} \alpha(\underline{v})|\Psi(\underline{v})|^2$$

Notice that $\Psi(\underline{v})$ is well defined due to the continuity condition in $H^1(\mathscr{G})$. One can prove that under Assumption 1 one has

$$\left|(\Psi, W\Psi) + \sum_{\underline{v} \in V} \alpha(\underline{v})|\Psi(\underline{v})|^2\right| \leqslant a\|\Psi'\|^2 + b\|\Psi\|^2, \qquad \text{with } 0 < a < 1,\ b > 0,$$

which, by KLMN theorem, implies that the form E^{lin} is closed and hence defines a selfadjoint operator. It is easy to prove that the corresponding operator coincides with H.

Let us define

$$-E_0 = \inf\left\{E^{lin}[\Psi],\ \Psi \in H^1(\mathscr{G}),\ \|\Psi\| = 1\right\}.$$

This corresponds to the bottom of the spectrum of H. A second assumption is needed in the proof of the main theorem.

Assumption 2 $\inf \sigma(H) := -E_0$ *is strictly negative*
Notice that this implies that $-E_0 < 0$ is an isolated simple eigenvalue. We denote by Φ_0 the corresponding normalized eigenfunction.

Equation (1) is well posed in $H^1(\mathscr{G})$ and the proof proceeds along well known lines as an application of Banach fixed point theorem. Global well-posedness then follows by conservation laws. We introduce the integral form of Eq. (1)

$$\Psi(t) \;=\; e^{-iHt}\Psi_0 + i\int_0^t e^{-iH(t-s)}|\Psi(s)|^{2\mu}\Psi(s)\,ds \tag{2}$$

Proposition 1 (Local Well-Posedness in $H^1(\mathscr{G})$) *Let $\mu > 0$ and Assumption 1 hold true. For any $\Psi_0 \in H^1(\mathscr{G})$, there exists $T > 0$ such that the Eq. (2) has a unique solution $\Psi \in C([0,T), H^1(\mathscr{G})) \cap C^1([0,T), H^1(\mathscr{G})^\star)$. Moreover, Eq. (2) has a maximal solution defined on an interval of the form $[0, T^\star)$, and the following "blow-up alternative" holds: either $T^\star = \infty$ or*

$$\lim_{t\to T^\star} \|\Psi(t)\|_{H^1(\mathscr{G})} \;=\; +\infty.$$

The nonlinear energy reads

$$\begin{aligned} E[\Psi] =& E^{lin}[\Psi] - \frac{1}{\mu+1}\|\Psi\|_{2\mu+2}^{2\mu+2} \\ =& \|\Psi'\|^2 + (\Psi, W\Psi) + \sum_{\underline{v}\in V}\alpha(\underline{v})|\Psi(\underline{v})|^2 - \frac{1}{\mu+1}\|\Psi\|_{2\mu+2}^{2\mu+2} \end{aligned}$$

and it is defined on $H^1(\mathscr{G})$. The mass functional is given by

$$M[\Psi] = \|\Psi\|^2.$$

Proposition 2 (Conservation Laws) *Let $\mu > 0$. For any solution $\Psi \in C^0([0,T), H^1(\mathscr{G})) \cap C^1([0,T), H^1(\mathscr{G})^\star)$ to the problem (2), the following conservation laws hold at any time t:*

$$M[\Psi(t)] \;= M[\Psi(0)], \qquad E[\Psi(t)] \;=\; E[\Psi(0)].$$

Proposition 3 (Global Well-Posedness) *Let $0 < \mu < 2$. For any $\Psi_0 \in H^1(\mathscr{G})$, the Eq. (2) has a unique solution $\Psi \in C^0([0,\infty), H^1(\mathscr{G})) \cap C^1([0,\infty), H^1(\mathscr{G})^\star)$.*

The main theorem in [18] gives the existence of nonlinear ground state under the above assumptions.

Theorem 1 *Let* $0 < \mu < 2$ *and consider on a graph* $\mathscr{G}$ *the following minimization problem:*

$$-\nu = \inf\{E[\Psi] \ s.t. \ \Psi \in H^1(\mathscr{G}),\ M[\Psi] = m\}. \tag{3}$$

If Assumptions 1, and 2 hold true, then $mE_0 < \nu < +\infty$ *for any* $m > 0$. *Moreover, there exists* $m^* > 0$ *such that for* $0 < m < m^*$ *there exists* $\hat{\Psi} \in H^1(\mathscr{G})$*, with* $M[\hat{\Psi}] = m$*, such that* $E[\hat{\Psi}] = -\nu$.

Notice that by standard arguments $\hat{\Psi}$ is orbitally stable, see [19]. We make some comments on the assumptions and then we sketch some ideas of the proof.

We remark that if $\mathscr{G}$ is a compact connected graph without infinite edges, the minimization problem (3) admits a solution whenever the energy functional $E[\Psi]$ is bounded from below.

Assumption 1 is a rather weak hypothesis which is sufficient to guarantee that E^{lin} is the quadratic form of a selfadjoint operator bounded from below.

Assumption 2 assures existence of a unique *linear* ground state and it is satisfied in many relevant examples, such as the following:

(a) No delta terms, i.e. $\alpha(\underline{v}) = 0$ for all $\underline{v}$ (also called Kirchhoff boundary conditions at vertices, see, e.g. [28]) and a sufficiently well behaved and decaying external potential attractive in the mean, i.e. such that $\int_{\mathscr{G}} W < 0$. In the pure Kirchhoff case (with no potentials) an extensive analysis of NLS with power nonlinearity has been given in the recent papers [8, 11], where in particular it is shown that existence of a ground state for subcritical nonlinearity holds true only in some exceptional cases, the simplest one being the tadpole graph [17, 32]. Here we show that summing a small negative potential restores the ground state generically.
(b) Absence of potential term and delta interactions negative in the mean: $\sum_{\underline{v}\in V} \alpha(\underline{v}) < 0$ (Se also [20] for an explicit example in this case).
(c) A mixing of the two: delta interaction at the vertices and well behaved potentials with negative potential energy: $\sum_{\underline{v}\in V} \alpha(\underline{v}) + \int_{\mathscr{G}} W < 0$.

Notice that at the level of quadratic form and in this one dimensional problem, strictly speaking, one could consider on the same footing both the delta terms and the regular potential term. We have a preference to keep separate the two contributions because this is the usual way they are treated in quantum graph literature.

Assumption 1 with the additional request that the potential W is relatively compact with respect to the laplacian on the graph (Kirchhoff or delta boundary conditions or a mixing of the two) assures that the Hamiltonian H admits an essential spectrum $\sigma_e(H) = [0, +\infty)$. So that, with this additional condition, a necessary hypothesis for Assumption 2 be satisfied is that at least a negative eigenvalue exists. It is straightforward to prove, considering a trial function constant on the compact part of the graph and smoothly vanishing at infinity that if $\sum_{\underline{v}\in V}|\alpha(\underline{v})| + \int_{\mathscr{G}} W$ is negative the quadratic form is negative on this trial function and so a negative eigenvalue exists. Moreover the delta interactions contribute at most with a finite number of eigenvalues and the same holds true if W_{-} is vanishing sufficiently fast at infinity. The additional request $\int_{\mathscr{G}} W(\underline{x})(1+|\underline{x}|)d\underline{x} < \infty$, as in the line or half line cases is sufficient to guarantee that the discrete spectrum is finite. In particular $-E_0 < 0$ is an isolated eigenvalue.

The non degeneracy of the principal eigenvalue is a subtler problem. When a ground state exists this property is assured by and is equivalent to the fact that the heat semigroup $S(t) = \exp(-tH)$ associated to H is positivity improving (see [34, Theorem XIII.44]). Moreover, a positivity preserving heat semigroup $S(t)$ is positivity improving, its generator has no ground state degeneracy and its ground state is positive if and only if $S(t)$ is irreducible. The Hamiltonian operator H_0, corresponding to the operator H with $W = 0$ and $\alpha(\underline{v}) \equiv 0$ generates a positive improving heat semigroup, see [25, 26]. This property is recovered for H by a standard approximation argument. We add, by way of information, that simplicity of *all* eigenvalues of quantum graph with delta interactions at vertices can be shown to be a generic property up to changing edge lengths and intensity of delta interactions, and again in absence of tadpoles (see [16] for details).

The main tool of the proof is an adaptation of concentration compactness lemma to the considered class of graphs. Notice that the translation invariance of the domain is broken and this forces a more detailed analysis of the Compact case which is split into Convergence and Runaway.

Let $d(\underline{x},\underline{y})$ be the distance between two points of the graph, defined as the infimum of the length of the paths connecting $\underline{x}$ to $\underline{y}$ and let $B(\underline{y},t)$ be the open ball of radius t and center $\underline{y}$

$$B(\underline{y},t) := \{\underline{x} \in \mathscr{G} \text{ s.t. } d(\underline{x},\underline{y}) < t\}.$$

For any function $\Psi \in L^2$ and $t \geqslant 0$ we define the concentration function $\rho(\Psi,t)$ as

$$\rho(\Psi,t) = \sup_{\underline{y}\in\mathscr{G}} \|\Psi\|^2_{B(\underline{y},t)} .$$

For any sequence $\Psi_n \in L^2$ we define the concentrated mass parameter τ as

$$\tau = \lim_{t\to\infty} \liminf_{n\to\infty} \rho(\Psi_n,t) .$$

The parameter τ plays a key role in the concentration compactness lemma because it distinguishes the occurrence of vanishing, dichotomy or compactness in $H^1(\mathscr{G})$-bounded sequences.

Lemma 1 (Concentration Compactness) *Let $m > 0$ and $\{\Psi_n\}_{n\in\mathbb{N}}$ be such that: $\Psi_n \in H^1(\mathscr{G})$,*

$$M[\Psi_n] \to m \quad as \quad n \to \infty\,,$$

$$\sup_{n\in\mathbb{N}} \|\Psi_n'\| < \infty\,.$$

Then there exists a subsequence $\{\Psi_{n_k}\}_{k\in\mathbb{N}}$ such that:

- *i) (Compactness) If $\tau = m$, at least one of the two following cases occurs:*
  - *i_1) (Convergence) There exists a function $\Psi \in H^1(\mathscr{G})$ such that $\Psi_{n_k} \to \Psi$ in L^p as $k \to \infty$ for all $2 \leqslant p \leqslant \infty$.*
  - *i_2) (Runaway) There exists $e^* \in E^{ex}$, such that for any $t > 0$, and $2 \leqslant p \leqslant \infty$*

$$\lim_{k\to\infty}\left(\sum_{e\neq e^*} \|(\Psi_{n_k})_e\|^p_{L^p(I_e)} + \|(\Psi_{n_k})_{e^*}\|^p_{L^p((0,t))}\right) = 0.$$

- *ii) (Vanishing) If $\tau = 0$, then $\Psi_{n_k} \to 0$ in L^p as $k \to \infty$ for all $2 < p \leqslant \infty$.*
- *iii) (Dichotomy) If $0 < \tau < m$, then there exist two sequences $\{R_k\}_{k\in\mathbb{N}}$ and $\{S_k\}_{k\in\mathbb{N}}$ in $H^1(\mathscr{G})$ such that*

$$\text{supp } R_k \cap \text{supp } S_k = \emptyset$$

$$|R_k(\underline{x})| + |S_k(\underline{x})| \leqslant |\Psi_{n_k}(\underline{x})| \qquad \forall \underline{x} \in \mathscr{G}$$

$$\|R_k\|_{H^1(\mathscr{G})} + \|S_k\|_{H^1(\mathscr{G})} \leqslant c\|\Psi_{n_k}\|_{H^1(\mathscr{G})}$$

$$\lim_{k\to\infty} M[R_k] = \tau \qquad\qquad \lim_{k\to\infty} M[S_k] = m - \tau$$

$$\liminf_{k\to\infty}\left(\|\Psi_{n_k}'\|^2 - \|R_k'\|^2 - \|S_k'\|^2\right) \geqslant 0$$

$$\lim_{k\to\infty}\left(\|\Psi_{n_k}\|_p^p - \|R_k\|_p^p - \|S_k\|_p^p\right) = 0 \qquad 2 \leqslant p < \infty$$

$$\lim_{k\to\infty}\left\| |\Psi_{n_k}|^2 - |R_k|^2 - |S_k|^2 \right\|_\infty = 0.$$

The strategy of the proof is simple. We have to prove that a minimizing sequence $\{\Psi_n\}_{n\in\mathbb{N}}$ can not be Vanishing, Dychotomic and Runaway as in the Concentration Compactness Lemma. Then it is straightforward to prove Theorem 1 from the Convergent case.

Up to subsequence, Ψ_n satisfy the following lower bound:

$$\frac{1}{\mu+1}\|\Psi_n\|_{2\mu+2}^{2\mu+2} + (\Psi, W_-\Psi) + \sum_{\underline{v}\in V_-} |\alpha(\underline{v})||\Psi_n(\underline{v})|^2 \geqslant \frac{\nu}{2}\,.$$

where V_- is the set of vertices where $\alpha(\underline{v}) < 0$. This is sufficient to rule out the Vanishing and the Dichotomy case. In order to rule out the Runaway case a more detailed analysis is required.

First it is proved that the energy of a Runaway sequence admits a lower bound by $E_\infty = E_\infty(m, \mu)$ which provides a threshold. This energy is associated with the corresponding variational problem on the line, that is:

$$E_\infty = \inf\left\{ \frac{1}{2} \int_{\mathbb{R}} |\phi'(x)|^2 \, dx \right.$$
$$\left. - \frac{1}{2\mu + 2} \int_{\mathbb{R}} |\phi(x)|^{2\mu+2} \text{ s.t. } \phi \in H^1(\mathbb{R}) \, , \int_{\mathbb{R}} |\phi(x)|^2 dx = m \right\}$$

Such a value is a crucial threshold in the minimization problem: if we can exhibit a trial function with lower energy then the Runaway case does not occur. Otherwise we can not exclude that Ψ_n converges weakly to 0 and we expect that the minimizer $\hat{\Psi}$ does not exist. This lower bound is quite natural since in the Runaway case Ψ_n is localized a single edge farther and farther from the compact region and therefore its contribution is negligible. We can say in general that for minimizing sequence $\{\Psi_n\}$ there is a competition between the possibility of staying in the compact region and running away at infinity along a single edge. Intuitively if the potential well is sufficiently deep the first possibility is favored otherwise the second occurs. It turns out that it is sufficient to assume that the potential creates a negative eigenvalue for H in order to rule out the Runaway case.

In order to exhibit such a trial function one need some guess on the ground state. In [18] it has been provided by bifurcation analysis of stationary state equation

$$H\Phi_\omega - |\Phi_\omega|^{2\mu}\Phi_\omega = -\omega\Phi_\omega \qquad \Phi \in \mathscr{D}(H), \ \omega > 0, \tag{4}$$

It has been proved that for sufficiently small m there is a continuous branch of solutions Φ_ω of (4) bifurcating from the linear ground state Φ_0 that has lower energy than the threshold described above and therefore the Runaway case does not happen and we are in the convergent case. Assumption 2 allows to apply bifurcation theory from an eigenvalue in its easiest version and to construct the nonlinear ground state. We stress that there is no obstruction in principle to consider bifurcation from a degenerate eigenvalue but we prefer to avoid unnecessary complications. Moreover the ground state is an element of such branch of stationary states.

3 Comparison with Other Results

In this section we compare Theorem 1 with other similar recent results in the literature. First of all notice that it ensures the existence of an absolute minimum just for an interval of masses. This is due to the nature of the problem and not to technical limitations as the results in [7] show. We comment on such results.

In [7] the same variational problem as in Theorem 1 is considered but in a simpler setting. First no external potential is present and then the underlying graph is a star graph, N half-lines with a common vertex, with an attractive δ-interaction of strength α in the vertex. Similar results are obtained.

Theorem 2 *Let m^{**} be defined by*

$$m^{**} = 2\frac{(\mu+1)^{1/\mu}}{\mu}\left(\frac{|\alpha|}{N}\right)^{\frac{2-\mu}{\mu}}\int_0^1 (1-t^2)^{\frac{1}{\mu}-1}\,dt.$$

Let $\alpha < 0$ and assume $m \leqslant m^{**}$ and $0 < \mu < 2$. Define

$$-\nu = \inf\{E[\Psi] \text{ s.t. } \Psi \in \mathscr{E}\,,\ M[\Psi] = m\}\,,$$

then $0 < \nu < \infty$ and there exists $\hat{\Psi}$ such that $M[\hat{\Psi}] = m$ and $E[\hat{\Psi}] = -\nu$.

The explicit expression of $\hat{\Psi}$ and of any other critical points of the energy functional can be given. For any $\omega > 0$, we label the soliton profile on the real line as

$$\phi_\omega(x) = [(\mu+1)\omega]^{\frac{1}{2\mu}}\operatorname{sech}^{\frac{1}{\mu}}(\mu\sqrt{\omega}x). \tag{5}$$

For any $\alpha < 0, j = 0, \ldots, \left[\frac{N-1}{2}\right]$ ($[x]$ denoting the integer part of x) and $\omega > \frac{\alpha^2}{(N-2j)^2}$ we define $\Psi_{\omega,j}$ as

$$\left(\Phi_{\omega,j}\right)(x,i) = \begin{cases} \phi_\omega(x-a_j) & i = 1,\ldots,j \\ \phi_\omega(x+a_j) & i = j+1,\ldots,N \end{cases} \tag{6}$$

with

$$a_j = \frac{1}{\mu\sqrt{\omega}}\operatorname{arctanh}\left(\frac{|\alpha|}{(N-2j)\sqrt{\omega}}\right). \tag{7}$$

The functions $\Phi_{\omega,j} \in \mathscr{D}(H)$ and are solutions of the stationary equation

$$H\Phi_\omega - |\Phi_\omega|^{2\mu}\Phi_\omega = -\omega\Phi_\omega. \tag{8}$$

We say that $\Phi_{\omega,j}$ has a "bump" (resp. a "tail") on the edge i if $\left(\Phi_{\omega,j}\right)(x,i)$ is of the form $\phi_\omega(x-a_j)$ (resp. $\phi_\omega(x+a_j)$). The index j in $\Phi_{\omega,j}$ denotes the number of bumps of the state $\Phi_{\omega,j}$. For this reason, we refer to the stationary state $\Phi_{\omega,0}$ as the "N-tail state". We remark that the N-tail state is the only symmetric (i.e. invariant under permutation of the edges) solution of Eq. (8). For $j \geqslant 1$ there are $\binom{N}{j}$ distinct solutions obtained by formulae (6) and (7) by positioning the bumps on the edges in all the possible ways. For instance, if $N = 3$ then there are two stationary states, a three-tail state and a two-tail/one-bump state. They are shown in Fig. 2.

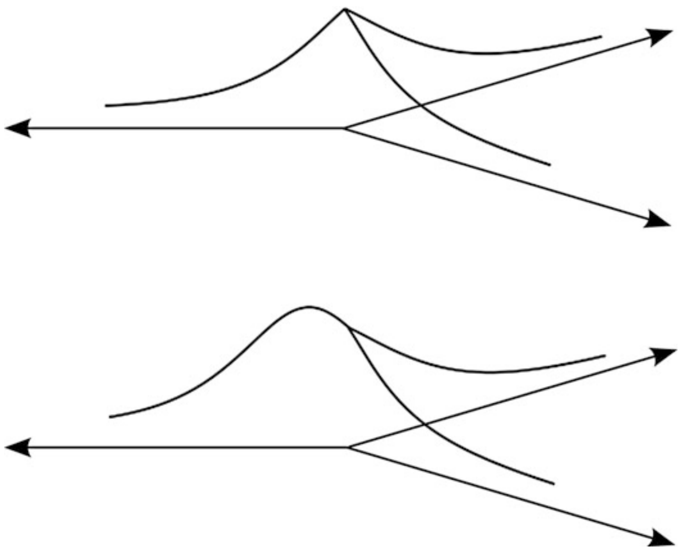

Fig. 2 Stationary states for $N = 3$, $\alpha < 0$

Theorem 3 *Let* $\alpha < 0$ *and assume* $m \leqslant m^{**}$ *and* $0 < \mu < 2$*; then the minimizer* $\hat{\Psi}$ *coincides with the N-tail state defined by* $\Phi_{\omega_0,0}$ *where* ω_0 *is chosen such that* $M[\Phi_{\omega_0,0}] = m$*.*

The explicit knowledge of the putative ground allows to obtain an explicit estimate of m^{**} in a straightforward way by giving a sufficient condition such that $E[\Psi_{\omega_0,0}] < E_\infty$ and the Runaway case is excluded. For $\mu = 1$ the energy of the ground state takes a simple expression and it is given by

$$E[\Phi_{\omega_0,0}] = -\frac{1}{24N^2} m(m^2 + 6m|\alpha| + 12|\alpha|^2)$$

while the threshold at infinity is given by

$$E_\infty = -\frac{m^3}{96}$$

Then if $N > 2$ and $m/|\alpha|$ is sufficiently big, we have that $E[\Phi_{\omega_0,0}] > E_\infty$ and no absolute minimizer exists since any other critical points has higher energy than the N-tail state. It is interesting noticing that in such limit $\Phi_{\omega_0,0}$ is still a stationary state and in facts it becomes a local minimizers for large m, see [10]. This concrete example shows that we can not expect to find a ground state for the NLS at any mass m. The case $N \leqslant 2$ is not included in this remark, indeed in the case of the line with a delta interaction, the existence of the ground state for every value of the mass was given in [5], which covers also other examples of point interactions, while an even more singular interaction is treated in [1].

One unusual feature of the star graph is the possibility to find all the critical points of the energy functional. This is due to the simplicity of the compact core, which is in this case just a point. If one consider a more general solution, when the compact case admit cycles (a closed path), a much more complex scenario is expected. In particular if the edges of a cycles are rationally dependent, the linear operator H admits infinitely many eigenvalues embedded in the continuum spectrum with corresponding eigenvectors localized in the compact core of the graph. Stationary states of the non linear problem may bifurcate from such eigenvalues of the linear problem. This phenomenon is observed in [17] where the stationary equation is considered for a cubic NLS on a tadpole graph.

$$H\Phi_\omega - |\Phi_\omega|^{2\mu}\Phi_\omega = -\omega\Phi_\omega \qquad \Phi \in \mathscr{D}(H), \tag{9}$$

A tadpole is a cycle with one vertex and one infinite edge, see Fig. 3. A Kirchhoff boundary condition is considered in the vertex. In the cubic case, solutions of (9) in compact region, i.e. the cycle, are written in term of Jacobi elliptic functions. The Hamiltonian admits $\lambda_n = (n\pi/L)^2$ as eigenvalues and the corresponding eigenvectors are localized on the head of the tadpole. Two families of stationary states are found. The first family called cn-solutions is infinite for every ω and is made by solutions $\Phi_{\omega,n}$ of (9) which bifurcate from the vacuum as ω crosses λ_n and are localized on the head of the tadpole. Moreover each branch of cn-solution $\Phi_{\omega,n}$ has an unexpected secondary bifurcation at $\omega = 0$ splitting into $\Phi^+_{\omega,n}$ and $\Phi^-_{\omega,n}$; this related to the presence of zero energy resonance of H. See Fig. 4 for a plot of the first elements of this family and for the secondary bifurcation of an element. The second family called dn-solutions and denoted by $\Xi_{\omega,n,1}$ (left) and $\Xi_{\omega,n,2}$,exist only for $\omega < 0$ and it is finite although the number of existing dn-solutions depend on ω. They are non zero everywhere and have no linear counterpart. See Fig. 5 for a plot of the first elements of this family. The tadpole graph shows that it would be extremely difficult for a general graph to have even a partial picture of the nonlinear spectrum, that is the set of critical points of the energy functional, although it is expected that they influence the propagation in the time dependent problem, see e.g. [24]. The analysis stationary states for general graphs in a suitable regime with weak nonlinearity has been carried out in [22] and [23].

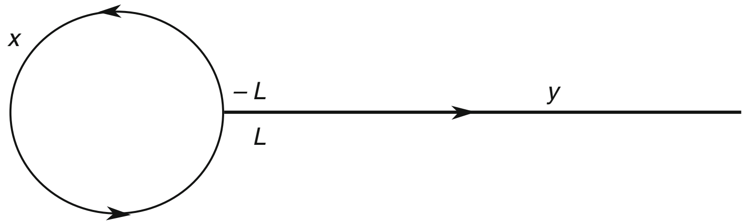

Fig. 3 Tadpole graph

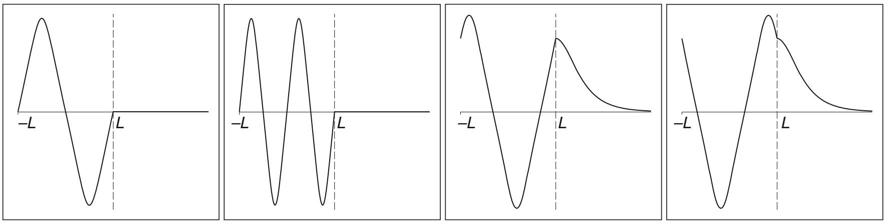

Fig. 4 *Left*: plots of representatives of cn-state $\Phi_{\omega,1}$ (*left*) and $\Phi_{\omega,2}$ (*right*). *Right*: plots of representatives of cn-state $\Phi^{+}_{\omega,1}$ (*left*) and $\Phi^{-}_{\omega,1}$ (*right*). On the *left* of the horizontal axis the ring $[-L, L]$; on the *right* the halfline

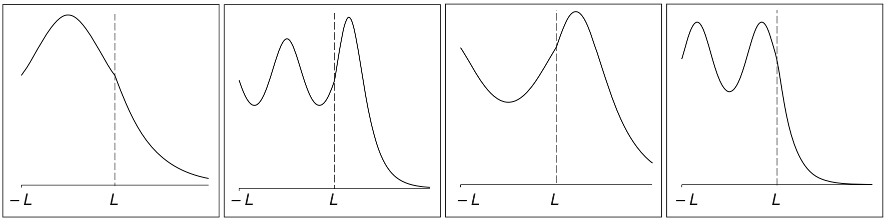

Fig. 5 *Left*: plots of representatives of dn-state $\Xi_{\omega,0,1}$ (*left*) and $\Xi_{\omega,0,2}$ (*right*). *Right*: plots of representatives of dn-state $\Xi_{\omega,1,1}$ (*left*) and $\Xi_{\omega,1,2}$ (*right*)

The ground state for the NLS on a general graph, like in Theorem 1, with Kirchhoff boundary condition, i.e. $\alpha(\underline{v}) = 0$, and no potential W, has been studied in a series of detailed papers, see [8, 9, 11]. It is clear that in this case the main hypothesis of Theorem 1, namely Assumption 2, is not satisfied since $H > 0$ and no negative eigenvalue is possible. In this setting there is no negative potential favoring Convergence over Runaway for a minimizing sequence and therefore the existence of ground state is not expected. They prove that for a very large class of graphs this the case, see [8]:

Theorem 4 *Assume that every point of $\mathcal{G}$ lies in a path connecting different vertices at infinity, then $-\nu = E_\infty$ and it is not achieved unless $\mathcal{G}$ is a special class of graphs called " bubble tower".*

These techniques and these results seem to be limited only to the Kirchhoff case. Indeed if we perturb a single vertex $\underline{v}$ such that $\alpha(\underline{v}) < 0$ and 0 otherwise, it is straightforward to prove that Assumption 2 is satisfied and Theorem 1 holds true, therefore a ground state exists.

It is also proved in [11] that if the topological assumption in Theorem 4 is violated, for certain graphs the a minimizer may exist depending on m. One example of such graph is the tadpole graph described above due to the presence of single half-line.

A second example is a star graph with a edge of length l. Notice this situation is qualitatively different from the situation considered in [7]. The reason is that, when looking for stationary states, one has a Neumann boundary condition in the vertex of degree one instead of Dirichlet one. Therefore we do not expect that the minimizer, for instance, approaches the N-tail state of [7] as $l \to \infty$. Indeed they prove that the ground state exists for sufficiently large masses which is the opposite of Theorem 2.

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Self-Adjoint Extensions of Dirac Operator with Coulomb Potential

Matteo Gallone

Abstract In this note we give a concise review of the present state-of-art for the problem of self-adjoint realisations for the Dirac operator with a Coulomb-like singular scalar potential $V(\mathbf{x}) = \phi(\mathbf{x}) I_4$. We try to follow the historical and conceptual path that leads to the present understanding of the problem and to highlight the techniques employed and the main ideas. In the final part we outline a few major open questions that concern the topical problem of the multiplicity of self-adjoint realisations of the model, and which are worth addressing in the future.

Keywords Dirac-Coulomb operator • Distinguished self-adjoint extension • Self-adjoint extensions • von Neumann extension theory

1 Introduction

In relativistic quantum mechanics one is interested in the study of Dirac equation, a partial differential equation that describes the dynamics of a $\frac{1}{2}$–spin fermion. The phase space of the physical system is the Hilbert space $\mathscr{L}^2 := L^2(\mathbb{R}^3, \mathbb{C}^4, \mathrm{d}^3 x)$ which is

$$\mathscr{L}^2 := \left\{ u \,|\, u : \mathbb{R}^3 \to \mathbb{C}^4,\ \|u\|_{\mathscr{L}^2} < \infty \right\}, \tag{1}$$

where if $u = (u_1, u_2, u_3, u_4)$, with $u_j : \mathbb{R}^3 \to \mathbb{C}$, $\|u\|^2_{\mathscr{L}^2} = \int_{\mathbb{R}^3} \sum_{j=1}^4 |u_j(\mathbf{x})|^2 \, \mathrm{d}^3 x$.

The minimal Dirac operator is defined by

$$T = \alpha \cdot \mathbf{p} + \beta + V(\mathbf{x}) \tag{2}$$

on the compactly supported smooth functions:

$$\mathscr{D}(T) = \mathscr{C}_c^\infty := C_c^\infty(\mathbb{R}^3 \setminus \{0\}; \mathbb{C}^4), \tag{3}$$

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A. Michelangeli, G. Dell'Antonio (eds.), *Advances in Quantum Mechanics*,
Springer INdAM Series 18, DOI 10.1007/978-3-319-58904-6_10

where $\mathbf{p} = -i\nabla$ is the momentum operator, $\alpha = (\alpha_1, \alpha_2, \alpha_3)$, α_j and $\alpha_4 = \beta$ are 4×4 Hermitian matrices which satisfy the anti-commutation relation

$$\alpha_j \alpha_k + \alpha_k \alpha_j = 2\delta_{jk} I_4, \tag{4}$$

I_n is the $n \times n$ identity matrix and $V(x)$ is a real 4×4 matrix valued function called *potential*. A standard form for the α matrices is the following

$$\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \tag{5}$$

where σ_j are the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{6}$$

In these notes we are interested in real scalar potentials of the form $V(\mathbf{x}) = \phi(\mathbf{x}) I_4$ which have a Coulomb-like singularity at the origin, namely $\lim_{\mathbf{x}\to 0} |\mathbf{x}|\phi(\mathbf{x}) = \nu \in \mathbb{R}$. For the sake of simplicity we will denote by T_0 the free Dirac operator and will refer to the operator $T = T_0 + V$ as the *Dirac-Coulomb* operator. A natural choice for ϕ is the Coulomb potential

$$\phi(\mathbf{x}) = \frac{\nu}{|\mathbf{x}|}, \tag{7}$$

and this means that one is modelling an electron subject to the electric field generated by ν positive charge in the origin.

In atomic models ν is related to the atomic number by

$$\nu = \frac{Z}{\alpha}, \tag{8}$$

where Z is the atomic number and α is the fine-structure constant $\alpha \sim 137$.

In the case of a multi-electron atom one can use some kind of screening approximation and an effective potential which is still Coulomb-like but it loses some properties like the spherical symmetry. This makes the study of self-adjoint extensions physically interesting also in the case of potentials with non spherical symmetry.

We collect in the following theorem what is known about the existence and uniqueness of self-adjoint extensions of the minimal Dirac-Coulomb operator [11, 14, 22–24, 26, 29].

Theorem 1 (Self-Adjoint Extensions of the Minimal Dirac-Coulomb Operator) *Let $T = T_0 + V$ be a Dirac-Coulomb operator defined on $\mathscr{C}_c^\infty$ with $V(\mathbf{x}) = \phi(\mathbf{x})I_4$ and*

$$\lim_{\mathbf{x}\to 0} |\mathbf{x}|\phi(\mathbf{x}) = \nu. \tag{9}$$

Then:

i) if $|\nu| < \frac{\sqrt{3}}{2}$, then the operator T is essentially self-adjoint and its unique self-adjoint extension has domain

$$\mathscr{D}(\bar{T}) = \mathscr{H}^1 := H^1(\mathbb{R}^3, \mathbb{C}^4, \mathrm{d}^3x). \tag{10}$$

ii) If $\frac{\sqrt{3}}{2} < |\nu| < 1$, then the operator T has infinitely many self-adjoint extensions and if $\phi(\mathbf{x})$ is bounded below or above there exists a unique distinguished extension T_d with the properties

$$\mathscr{D}(T_d) \subset \mathscr{D}(|\mathbf{x}|^{-1/2}), \qquad \mathscr{D}(T_d) \subset \mathscr{D}(|T_0|^{1/2}). \tag{11}$$

iii) If $|\nu| > 1$, then there are infinitely many self-adjoint extensions of T.

The reason why in the regime $\frac{\sqrt{3}}{2} < |\nu| < 1$ we call T_d distinguished is that physically the condition (11) is a requirement for the functions in $\mathscr{D}(T_d)$ to have a finite kinetic and potential energy. It is also notice-worthy that T_d is the unique self-adjoint extension with this property (see Sect. 3.2).

Another important remark is on the threshold value $|\nu| = \frac{\sqrt{3}}{2}$. In fact, in this case, it is not possible to determine whereas T is essentially self-adjoint or not without any further information on V (see [29] for more details). In the special case of the pure Coulomb potential (7) for the choice $|\nu| = \frac{\sqrt{3}}{2}$ the operator T is essentially self-adjoint.

Due to these reasons, in the literature one usually refers to (i) as the *regular regime*, to (ii) as the *transitory regime*, and to (iii) as the *critical regime*.

The first step in the study of self-adjoint extensions is the computation of the deficiency indices of the Dirac-Coulomb operator: we discuss it in Sect. 2. In Sect. 3 we place the study of the self-adjoint extensions of Dirac-Coulomb operators into a historical perspective from Kato's paper in 1951 up to recent works. This includes also the sketch of some key proofs, with no pretension of completeness. In Sect. 4 we present what is known about the classification of self-adjoint extensions of the Dirac operator. Last, in Sect. 5 we present some questions that, to our opinion, are more relevant and deserve further investigations.

2 Deficiency Indices

In this section we compute the deficiency indices for the Dirac-Coulomb operator. We recall that given a densely defined symmetric operator T its deficiency indices are

$$n_{\pm} := \dim \ker(T^* \mp i). \tag{12}$$

In a sense they measure 'how far' the operator T is from being self-adjoint. More precisely, by a well-known result (see [18] Corollary to Theorem X.2), a densely defined symmetric operator admits non-trivial self-adjoint extensions if and only if the deficiency indices are equal and different from zero: $n_+ = n_- \neq 0$. If this is true and $n_+ < \infty$, then all the self-adjoint extensions of T are parametrized by n_+^2 real parameters. It is therefore very natural to begin this review on self-adjoint extensions of Dirac-Coulomb operator with the computation of the deficiency indices.

Theorem 2 ([26], Theorem 6.9) *Let T be the Dirac operator with Coulomb potential with $V(x) = \frac{\nu}{|x|} I_4$ defined on $\mathscr{C}_c^\infty$. Then the deficiency indices are*

i) $(0,0)$ *if* $|\nu| \leq \frac{\sqrt{3}}{2}$;
ii) $(2n(n+1), 2n(n+1))$ *if* $\sqrt{n^2 - \frac{1}{4}} < |\nu| \leq \sqrt{(1+n)^2 - \frac{1}{4}}$ *with* $n \in \mathbb{N}$.

Remark 1 The deficiency indices for the Dirac operator with scalar potential are the same even if we relax the hypothesis of spherical symmetry of the potential. In fact, the statement of the theorem remains unchanged except for the fact that the inequalities become all strict. In order to compute the deficiency indices for $\nu = \sqrt{n^2 - \frac{1}{4}}$ in the general case of non spherical symmetry one needs additional information on the potential (see [29] Theorem 4.2).

Proof By passing to polar coordinates and denoting with $\mathrm{d}\Omega$ the surface measure of the unit sphere we obtain an isomorphism

$$U : L^2(\mathbb{R}^3, \mathbb{C}, \mathrm{d}^3x) \to L^2((0,\infty), \mathbb{C}, \mathrm{d}r) \otimes L^2(\mathbb{S}^2, \mathbb{C}, \mathrm{d}\Omega) \tag{13}$$

by setting for each $\Psi \in L^2(\mathbb{R}^3, \mathbb{C}, \mathrm{d}^3x)$

$$(U\Psi)(r, \vartheta, \varphi) = r\Psi(\mathbf{x}(r, \vartheta, \varphi)). \tag{14}$$

The isomorphism can be extended to $\mathscr{L}^2$ component-wise and it will be denoted with the same symbol. Under this transformation the free Dirac operator takes the form

$$UT_0U^* = -\mathrm{i}(\alpha \cdot \hat{\mathbf{r}}) \left(\frac{\partial}{\partial r} - \frac{2}{r} \mathbf{S} \cdot \mathbf{L} \right) + \beta. \tag{15}$$

Here $\mathbf{L} = \mathbf{x} \times \mathbf{p}$ denotes the angular momentum operator, $\mathbf{S} = -\frac{1}{4}\alpha \times \alpha$ the spin operator and $\hat{\mathbf{r}}$ is the radial versor.

A direct computation shows that the operator $\mathbf{S} \cdot \mathbf{L}$ commutes with the free Dirac operator UT_0U^*. To proceed in the analysis it is convenient to introduce the operator $K = 2\beta(\mathbf{S} \cdot \mathbf{L} + 1)$ in order to re-write the free Dirac operator as

$$UT_0U^* = -\mathrm{i}(\alpha \cdot \hat{\mathbf{r}}) \left(\frac{\partial}{\partial r} + \frac{1}{r} - \frac{1}{r}\beta K \right) + \beta. \tag{16}$$

Denoting with $\mathbf{J} = \mathbf{L} + \mathbf{S}$ the total angular momentum operator, it is possible to show that the operator K commutes with J^2 and with the third component of the total angular momentum operator J_3. Moreover, it is possible to find a common basis of infinitely differentiable orthonormal eigenfunctions on $L^2(\mathbb{S}^2, \mathbb{C}^4, \mathrm{d}\Omega)$ and to prove that all these operators have pure point spectrum (see [26] appendix to section 1).

The Hilbert space decomposes into the direct sum of 2-dimensional spaces

$$L^2(\mathbb{S}^2, \mathbb{C}^4, \mathrm{d}\Omega) = \bigoplus_{j \in \mathbb{N}+\frac{1}{2}} \bigoplus_{m_j=-j}^{j} \bigoplus_{\kappa_j = \pm(j+\frac{1}{2})} \mathscr{K}_{m_j,\kappa_j}, \tag{17}$$

where $\mathscr{K}_{m_j,\kappa_j} = \mathrm{span}\{\Phi^+_{m_j,\kappa_j}, \Phi^-_{m_j,\kappa_j}\}$ and $\Phi^\pm_{\kappa_j,m_j}$ are smooth common eigenfunctions of J^2, K, J_3 with eigenvalues $j(j+1)$, κ_j and m_j respectively.

Now each vector $\psi \in U^*\mathscr{C}_c^\infty$ can be written as

$$\psi(r, \vartheta, \varphi) = \frac{1}{r} \sum_{j,m_j,\kappa_j} \left(f^+_{m_j,\kappa_j}(r)\Phi^+_{m_j,\kappa_j}(\vartheta, \varphi) + f^-_{m_j,\kappa_j}(r)\Phi^-_{m_j,\kappa_j}(\vartheta, \varphi) \right) \tag{18}$$

with coefficient functions $f^\pm_{m_j,\kappa_j}(r) \in C_c^\infty((0, \infty))$. Hence, by putting together all the ingredients, we can compute the action of the radial Dirac-Coulomb operator on each reducing subspace $\mathscr{K}_{m_j,\kappa_j} \otimes C_c^\infty((0, \infty))$ as

$$t_{m_j,\kappa_j} = \begin{pmatrix} 1 + \frac{\nu}{r} & -\frac{d}{dr} + \frac{\kappa_j}{r} \\ \frac{d}{dr} + \frac{\kappa_j}{r} & -1 + \frac{\nu}{r} \end{pmatrix}, \tag{19}$$

and one is left with the computation of the deficiency indices for this ordinary differential operator.

Following Weidmann's argument we exploit a limit-point/limit-circle analysis. The differential operator t_{m_j,κ_j} is said to be in the *limit point case* at 0 (resp. at ∞) if for every $\lambda \in \mathbb{C}$ all solutions of $(t_{m_j,\kappa_j} - \lambda)u = 0$ are square integrable in $(0, 1)$ (resp. in $(1, \infty)$). The operator t_{m_j,κ_j} is said to be in the *limit circle case* at 0 (resp. at ∞) if for every $\lambda \in \mathbb{C}$ there is at least one solution of $(t_{m_j,\kappa_j} - \lambda)u = 0$ which is not square integrable in $(0, 1)$ (resp. in $(1, \infty)$).

Once we know if t_{m_j,κ_j} is in the limit circle case or in the limit point case the following general theorem gives us the deficiency indices.

Theorem 3 ([26], Theorem 5.7) *The deficiency indices of* t_{m_j,κ_j} *are*

i) $(2,2)$ *if* t_{m_j,κ_j} *is in limit circle case at both* 0 *and* ∞*;*
ii) $(1,1)$ *if* t_{m_j,κ_j} *is in limit circle case at one end point and in limit point case at the other;*
iii) $(0,0)$ *if* t_{m_j,κ_j} *is in limit point case at both* 0 *and* ∞*.*

By Weyl's alternative theorem (see [26] Theorem 5.6), either for every $\lambda \in \mathbb{C}$ all solutions of $(t_{m_j,\kappa_j} - \lambda)u = 0$ are square integrable in $(0,1)$ (resp. in $(1,\infty)$), or for every $\lambda \in \mathbb{C} \setminus \mathbb{R}$ there exists a unique (up to a multiplicative constant) solution u of $(t_{m_j,\kappa_j} - \lambda)u = 0$ which is square integrable in $(0,1)$ (resp. in $(1,\infty)$). Therefore, since no third option is possible, it is sufficient to check whether both the solutions of $t_{m_j,\kappa_j}u = 0$ are square integrable in $(0,1)$ and $(1,\infty)$.

To check if t_{m_j,κ_j} is in the limit-point or in the limit-circle case we consider the operator $(t_{m_j,\kappa_j} - \beta)$. The subtraction of a bounded operator does not change the computation of the deficiency indices. Choosing $\lambda = 0$, the equation to be solved is $(t_{m_j,\kappa_j} - \beta)u = 0$. Its solutions are

$$u(r) = \begin{pmatrix} u^+(r) \\ u^-(r) \end{pmatrix} = \begin{pmatrix} \pm\sqrt{\kappa_j^2 - \nu^2} - \kappa_j \\ \nu \end{pmatrix} r^{\pm\sqrt{\kappa_j^2-\nu^2}}. \tag{20}$$

From this explicit expression we see that the solution with positive exponent cannot be square integrable in $(1,\infty)$ and hence independently of the parameters κ_j and ν the operator is always in the limit point case at infinity.

The solution with positive exponent is always square integrable in $(0,1)$ while the one with negative square root is square integrable near zero if and only if

$$-2\sqrt{\kappa_j^2 - \nu^2} \leq -1, \tag{21}$$

which means

$$\nu^2 \leq \kappa_j^2 - \frac{1}{4}. \tag{22}$$

Then if ν satisfies (22), the operator is in the limit point case at both endpoints. By Theorem 3, if (22) holds the deficiency indices of the operator are $(0,0)$, otherwise the deficiency indices of the operator are $(1,1)$.

To compute the deficiency indices of the full operator we have to count how many reduced operators are not essentially self-adjoint. Explicitly,

$$n_\pm = \sum_{j\in\mathbb{N}+\frac{1}{2}} \sum_{m_j=-j}^{j} \sum_{\kappa_j=\pm(j+\frac{1}{2})} \begin{cases} 1 & \text{if} \quad \nu^2 > \kappa_j - \frac{1}{4} \\ 0 & \text{else} \end{cases}. \tag{23}$$

Let n be the integer such that $n^2 - \frac{1}{4} < \nu^2 \leq (n+1)^2 - \frac{1}{4}$. We obtain

$$n_{\pm} = \sum_{j \in \mathbb{N}+\frac{1}{2}}^{n-\frac{1}{2}} \sum_{m_j=-j}^{j} 2 = 2n(n+1). \tag{24}$$

3 Potential with Coulomb-Like Singularity

In this section we review the historical path that, together with the results in the previous section, led to the present understanding on the existence and uniqueness of self-adjoint extensions of the minimal Dirac-Coulomb operator.

Conceptually and historically the two main questions addressed so far, and that we are going to analyse are:

1. Is the operator $T_0 + V$ essentially self-adjoint?
2. If it is not, is there a *special* self-adjoint extension which is physically relevant?

The technique employed in answering the first question is essentially a perturbative argument based on the Kato-Rellich theorem and it is addressed in the first subsection.

The second question presents a wider range of answers and many authors provided different meaningful special extensions. Only at a later stage they recognized that, under some hypothesis, they were referring to the same operator. This subject is addressed in the second subsection.

3.1 Essential Self-Adjointness via Kato-Rellich Theorem

One of the first proofs of the essential self-adjointness for the Dirac-Coulomb operator is due to Kato in 1951 as a direct application of the Kato-Rellich theorem. Despite the simplicity of the proof, this does not cover the whole range of the parameter ν on which the Dirac-Coulomb operator is essentially self-adjoint.

Some years later two different approaches based on the same theorem were developed in order to cover the range $[0, \frac{\sqrt{3}}{2}]$: the first one, due to Rejtö and Gustafsson [10, 19] aimed to weaken its hypotheses, the other one due to Schminke [22] uses the original theorem. Instead of looking to V as a perturbation of T_0 he introduced an operator C and considered $T_0 + V = (T_0 + C) + (V - C)$. To prove the essential self-adjointness of $T_0 + V$ he proved separately the essential self-adjointness of $T_0 + C$ and looked at $V - C$ as a perturbation satisfying the hypothesis of Kato-Rellich.

Several other works dealt with the same problem, among which we mention [5, 7, 15, 20, 21, 25]. For a self-contained conceptual review we present in detail only the above-mentioned ones of Rejtö-Gustaffson and Schmincke.

Since it will play a central role in this subsection, we recall the classical statement of the Kato-Rellich theorem.

Theorem 4 (Kato-Rellich) *Suppose that A is an essentially self-adjoint operator, B is a symmetric operator that is A-bounded with relative bound $a < 1$, namely*

i) $\mathscr{D}(B) \supset \mathscr{D}(A)$;
ii) For some $a < 1$, $b \in \mathbb{R}$ *and for all* $\varphi \in \mathscr{D}(A)$,

$$\|B\varphi\| \leq a\|A\varphi\| + b\|\varphi\|. \tag{25}$$

Then $\overline{A+B}$ is self-adjoint on $\mathscr{D}(\bar{A})$ and essentially self-adjoint on any core of A.

Let us start with surveying Kato's proof from [12, 13]. The starting point is the well-known Hardy inequality (see [18] section X.2 p.169)

$$\|\mathbf{p}u\|^2 \geq \frac{1}{4}\|r^{-1}u\|^2, \qquad \forall u \in C_c^\infty(\mathbb{R}^3). \tag{26}$$

By using the properties of the α matrices we get the identity

$$\|T_0 u\|^2 = \|\mathbf{p}u\|^2 + \langle(\beta\boldsymbol{\alpha}\cdot\mathbf{p} + \boldsymbol{\alpha}\cdot\mathbf{p}\beta)u, u\rangle + \|u\|^2 = \|\mathbf{p}u\|^2 + \|u\|^2. \tag{27}$$

Thus, we see that if the potential is $|\phi(\mathbf{x})| \leq \frac{\nu}{|\mathbf{x}|}$, we get the following chain of inequalities

$$\|\mathbf{p}u\|^2 \geq \frac{1}{4}\|r^{-1}u\|^2 \geq \frac{1}{4\nu^2}\|\phi(\mathbf{x})u\|^2, \tag{28}$$

from which it follows that

$$\|\phi(\mathbf{x})u\| \leq 4\nu^2\|T_0 u\|^2 - 4\nu^2\|u\|^2. \tag{29}$$

If $\nu < \frac{1}{2}$, the hypotheses of the Kato-Rellich theorem are satisfied and one deduces that $T_0 + V$ is essentially self-adjoint and the domain of the unique self adjoint extension is

$$\mathscr{D}(\overline{T_0 + V}) = \mathscr{H}^1. \tag{30}$$

Remark 2 By using Wüst theorem (see [18] theorem X.14) one can cover the case $\nu = \frac{1}{2}$. However the information on the domain of the self-adjoint extension is lost.

Remark 3 The result is independent of the possible spherical symmetry and of precise matricial form of the potential: the conclusion holds if $\lim_{x\to 0}|x||V_{ij}(x)| < \frac{1}{2}$, where $i, j = 1, 2$ and V_{ij} are the entries of the matrix V.

Remark 4 Arai [1, 2] showed that by considering more general matrix-valued potentials of the form

$$V(x) = \frac{Z}{r} I_4 + \frac{\mathrm{i}}{r} \alpha \cdot \hat{\mathbf{r}} \beta b_1 + \frac{\beta}{r} b_2 \tag{31}$$

the necessary and sufficient condition for the essential self-adjointness is $(\kappa_j + b_1)^2 + b_2^2 \geq Z^2 + \frac{1}{4}$ and hence the threshold $\frac{1}{2}$ is optimal, in the sense that if V is in the form above and one of the entry of the matrix satisfies $|x||V_{ij}| > \frac{1}{2}$ then it is possible to choose Z, b_1, b_2 such that the operator is not essentially self-adjoint.

In a work from 1970, Rejtö [19] discussed the particular case of spherically symmetric Coulomb-like potentials. By denoting with $B(\mathscr{L}^2)$ the set of bounded operators on $\mathscr{L}^2$, the requirement on V for the operator $T_0 + V$ to be essentially self-adjoint on $\mathscr{C}_c^\infty$ boils down to asking that $\exists \mu_\pm$ in the upper/lower closed complex half plane such that

$$(1 - \bar{V}(\mu_\pm - \bar{A}_0)^{-1}) \in B(\mathscr{L}^2). \tag{32}$$

Proving that the Dirac operator with Coulomb interaction satisfies this hypothesis for $\nu \in [0, \frac{3}{4})$, he was able to show that under this condition such an operator is essentially self-adjoint and the domain of its self-adjoint extension is $\mathscr{H}^1$.

In fact [19] provides some sort of intermediate results that led to the more relevant work [10] by Gustaffson and Rejtö. In this relevant continuation they generalized further Kato-Rellich theorem and they were able to achieve the essential self-adjointness for the Dirac operator in the regime $\nu \in [0, \sqrt{3}/2)$.

Their generalization relies on Fredholm's theory, that we briefly recall here for the self-consistency of the presentation. A densely defined operator A in a Banach space $\mathscr{X}$ is said to be Fredholm if A is closed, $\operatorname{ran} A$ is closed, and both $\dim \ker A$ and $\dim \mathscr{X}/\operatorname{ran} T$ are finite. The index of a Fredholm operator A is the number $i(T) = \dim \ker A - \dim \mathscr{X}/\operatorname{ran} A$.

Theorem 5 ([10], Theorem 3.1, Generalized Kato-Rellich Theorem) *Let T_0 be essentially self-adjoint, V symmetric with $\mathscr{D}(V) \supset \mathscr{D}(T_0)$ where V is T_0-bounded. For each μ in the resolvent set of T_0 define the operator $A_\mu \in B(\mathscr{L}^2)$ by*

$$A_\mu := I - \bar{V}(\mu - \bar{T}_0)^{-1}. \tag{33}$$

Then the three conditions below

i) $T_0 + V$ *is essentially self-adjoint;*
ii) $\overline{T_0 + V} = \bar{T}_0 + \bar{V}$*;*
iii) $\mathscr{D}(\overline{T_0 + V}) = \mathscr{D}(\bar{T}_0)$*;*

hold if and only if there exists μ_+ in the closed upper half plane and μ_- in the closed lower half plane such that the operators $A_{\mu_\pm}$ are Fredholm of index zero.

Proof (Sketch) We start from the identity

$$\mu - \bar{T}_0 - \bar{V} = [I - \bar{V}(\mu - \bar{T}_0)^{-1}](\mu - \bar{T}_0). \tag{34}$$

Since $\mu \in \rho(T_0)$, $\mu - \bar{T}_0$ is Fredholm of index zero and since the composition of Fredholm operators is Fredholm and the index of the composition is the sum of the indices, by using a standard criterion of essential self-adjointness, we prove the sufficient condition.

The necessity follows using the same index-formula and the fact that if $A_1 A_2$ is Fredholm with A_2 Fredholm and A_1 closed, then A_1 is Fredholm and therefore by the above formula $A_{\pm i}$ is Fredholm of index 0.

Remark 5 This theorem includes the classical Kato-Rellich noting that with $\mu_\pm = \pm i\frac{a}{b}$ one has $\|\bar{V}(\mu_\pm - \bar{T}_0)^{-1}\| < 1$. Hence $A_{\mu_\pm}$ are invertible and therefore Fredholm of index zero.

The proof of the essential self-adjointness of the Dirac operator with Coulomb potential uses the following corollary:

Corollary 1 *If there exist μ_+ and μ_- as in the previous theorem such that $A_{\mu_\pm} = B_\pm + C_\pm$ where $B_\pm^{-1} \in B(\mathscr{L}^2)$ and $C_\pm$ are compact, then $T_0 + V$ is essentially self-adjoint and $\mathscr{D}(\overline{T_0 + V}) = \mathscr{D}(\bar{T}_0)$.*

Proof This corollary follows from the fact that an invertible operator is Fredholm of index zero and that this property is stable under compact perturbations.

By using the spherical symmetry and the decomposition of the Dirac operator Rejtö and Gustaffson prove that for $|\nu| \in [0, \frac{\sqrt{3}}{2})$ the hypothesis of Corollary 1 are satisfied and hence the spherically symmetric Dirac-Coulomb operator is essentially self-adjoint for that range of parameters.

In this respect the work of Schmincke [22] is of interest in that the same conclusion on essential self-adjointness was obtained *independently* of the spherical symmetry of the potential.

Theorem 6 ([22]) *Let $\phi \in L^2_{loc}(\mathbb{R}^3 \setminus \{0\}, \mathbb{R}, \mathrm{d}^3x)$ be a real-valued function that can be expressed as $\phi = \phi_1 + \phi_2$ with $\phi_1 \in C^0(\mathbb{R}^3 \setminus \{0\}, \mathbb{R})$ and $\phi_2 \in L^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{R}, \mathrm{d}^3x)$ with*

$$|\phi_1(\mathbf{x})| \leq \frac{\nu}{|\mathbf{x}|} \tag{35}$$

and $\nu \in [0, \frac{\sqrt{3}}{2})$. Then $T_0 + V$ is essentially self-adjoint.

The way Schmincke proves its result consists of using the standard Kato-Rellich theorem. He introduces a certain intercalary operator C in order to write $T_0 + V = (T_0 + C) + (V - C)$ and to regard $V - C$ as a small perturbation of $T_0 + C$.

More precisely he continues

$$C := \frac{1}{4}\left(a - \frac{1}{r}\right)\boldsymbol{\alpha}\cdot\hat{\mathbf{r}}, \qquad 1 < a < 3 \tag{36}$$

and $T_0 = \alpha \cdot \mathbf{p} + \beta$. He further introduces a bounded operator S_2 on which we omit the details. From these definitions it is clear that for $z \in \mathbb{C}$, $0 < |z| < 1$,

$$T_0 + V = (A + \beta + zC) + (V - zC - S_2) + S_2 = F + G + S_2. \tag{37}$$

With these definitions Schmincke proves that $\|Gu\|^2 \leq k\|Fu\|^2$ with $k < 1$ and hence Gu is F-bounded with a small bound. One can thus apply Kato-Rellich[1] to obtain that $T + V + S_2$ is essentially self-adjoint and, since S_2 is a bounded operator, this also implies the essentially self-adjointness of T.

3.2 *The Distinguished Self-Adjoint Extension*

As stated in Theorem 1, in the transitory regime there are infinitely many self-adjoint extensions of the minimal Dirac-Coulomb operator. Before considering their classification the main interest throughout the 1970s was the study of a *distinguished* extension characterized by being the most physically meaningful. The first work that introduced this particular self-adjoint extension is due to Schmincke [23] who obtained this extension by means of a multiplicative intercalary operator. This self-adjoint realisation is physically relevant because its domain is contained in the domain of the potential energy form and hence each function on the domain has a finite expectation value of the potential energy operator.

A second and more explicit construction of a distinguished self-adjoint extension of the minimal Dirac-Coulomb operator was found by Wüst [27, 28] by means of cut-off potentials. He built a sequence of self-adjoint operators that converges strongly in the operator graph topology to a self-adjoint extension of the minimal Dirac-Coulomb operator. Remarkably that the domain of this self-adjoint extension is also contained in the domain of the potential energy.

At that point it was not clear whether Wüst's and Schmincke's self-adjoint extensions were the same or not. The first attempt to look for a distinguished self-adjoint extension with a requirement of uniqueness was made by Nenciu [17] who found that there exists a unique self-adjoint extension of the minimal Dirac operator whose domain is contained in the domain of the kinetic energy form.

[1]Schmincke used a complex version of Kato-Rellich that deals with closed operators instead of self-adjoint ones. This is necessary because, in general, the z appearing in the proof is not real.

In 1979 Klaus and Wüst [14] proved that in the regime $\nu \in (\frac{\sqrt{3}}{2}, 1)$ if the potential ϕ is semi-bounded all the above mentioned distinguished self-adjoint extensions coincide.

Let us start with Schmincke's result.

Theorem 7 ([23], Theorems 2 and 3) *Let $\phi \in L^2_{loc}(\mathbb{R}^3 \setminus \{0\}, \mathbb{R}, d^3x)$ be a real-valued function such that $\phi = \phi_1 + \phi_2$ with ϕ_1 and ϕ_2 both real valued, $\phi_1 \in C^0(\mathbb{R}^3 \setminus \{0\})$, and $\phi_2 \in L^\infty(\mathbb{R}^3, \mathbb{R}, d^3x)$. Let $s \in [0, 1)$. Suppose there exists $k > 1$, $c > 1$ and $f \in C^1((0, \infty))$ positive valued and bounded from above by $\frac{1-s}{2c}$ such that*

$$\frac{1}{r^2}\left(f(r) + \frac{s}{2}\right)^2 \le k\left(|\phi_1(\mathbf{x})|^2 + \frac{1}{r^2}f^2(r)\right) \le \frac{1}{r^2}\left(f(r) + \frac{s+1}{2}\right)^2 + \frac{1}{r}f'(r). \tag{38}$$

Then there exists a bounded symmetric operator S such that

$$T_G := \left(\overline{r^{-\frac{s}{2}}}\right)\left(\overline{r^{\frac{s}{2}}(T-S)}\right) + \bar{S} \tag{39}$$

is an essential self-adjoint extension of T and $\forall m \in [\frac{1}{2}, 1 - \frac{s}{2}]$

$$\mathscr{D}(\overline{T}_G) = \mathscr{D}(T^*) \cap \mathscr{D}\left(\overline{r^{-m}}\right). \tag{40}$$

Remark 6 Note that in particular $\mathscr{D}(T_G) \subset \mathscr{D}\left(\overline{r^{-1/2}}\right)$, which physically means that all the functions in the domain of this distinguished self-adjoint extension have a finite expectation of the potential energy.

Schmincke proved this using a multiplicative intercalary operator. If $T = T_0 + V$ with T_0 essentially self-adjoint and if there exists a symmetric operator G satisfying suitable properties (see Theorem 1 in [23]), then

$$T_G := \overline{G^{-1}}\,\overline{GT} \tag{41}$$

is an essentially self-adjoint extension of T.

Noticeably in the case of Coulomb potential the assumptions of the theorem are satisfied when

$$1 - 4\nu^2 \le (1 - s^2) \le 4(1 - \nu^2), \tag{42}$$

which means $\nu < 1$.

Wüst, instead, showed that given a potential $\phi(\mathbf{x}) \in C^0(\mathbb{R}^3 \setminus \{0\})$ such that

$$|\phi(\mathbf{x})| \le \frac{\nu}{|\mathbf{x}|} \qquad |\nu| < 1, \tag{43}$$

if one fixes a positive constant $c > 0$ and defines

$$V_t(\mathbf{x}) := \begin{cases} V(\mathbf{x}) & |\mathbf{x}| \geq \frac{c}{t} \\ R(\mathbf{x}) & |\mathbf{x}| < \frac{c}{t}, \end{cases} \tag{44}$$

where R is chosen such that the components of V_t are continuous functions. If $V_t(\mathbf{x})$ is definitely monotone, the sequence of operators $T_t = T_0 + V_t$ g-converges to a self-adjoint operator T_g which is a self-adjoint extension of T with the property that

$$\mathscr{D}(T_g) \subset \mathscr{D}\left(\overline{r^{1/2}}\right). \tag{45}$$

In 1976 Nenciu [17] proposed an alternative distinguished self-adjoint extension T_N by requiring this extension to be the unique with the property that all the functions in its domain have finite kinetic energy, namely

$$\mathscr{D}(T_N) \subset \mathscr{D}(|\bar{T}_0|^{\frac{1}{2}}). \tag{46}$$

The precise result can be stated as follows.

Theorem 8 ([17], Theorem 5.1) *Let $w(t)$ be a decreasing function on $[0, \infty)$ such that $0 \leq w(t) \leq 1$, $\lim_{t\to\infty} w(t) = 0$, T_0 and V be a matrix-valued potential.*

If

i) $V(\mathbf{x}) = w(|\mathbf{x}|)W(\mathbf{x})$ *where W is a small perturbation of T_0, or*
ii) $V(\mathbf{x}) = V_1(\mathbf{x}) + V_2(\mathbf{x})$ *where V_1 is dominated by the Coulomb potential with coupling constant $\nu < 1$ and $V_2 = w(|\mathbf{x}|)W_2(\mathbf{x})$ where W_2 is non-singular,*

then

i) there exists a unique operator T_N such that

$$\mathscr{D}(T) \subset \mathscr{D}(|\overline{T}_0|^{\frac{1}{2}}); \tag{47}$$

ii) $\sigma_{ess}(T) \subset \sigma_{ess}(T_0)$.

The proof relies on a variant of Lax-Milgram lemma and has the inconvenience not to be constructive.

In 1979 Klaus and Wüst [14] showed that in the case of semi-bounded potential Wüst's and Nenciu's distinguished extensions actually coincide. This is an interesting fact both from a physical and from a mathematical point of view. Physically this coincidence means that the distinguished self-adjoint extension has the property of being the only one whose functions in the domain have finite potential *and* kinetic energy. From a mathematical point of view this overcomes the fact that Nenciu's method was not constructive and provides instead an explicit expression for its self-adjoint extension in terms of g-limit of T_t.

The identification of a certain *distinguished extension* was pushed further by Esteban and Loss [6] up to the value $\nu = 1$. In that paper they proposed to define the distinguished self-adjoint extension via Hardy-Dirac inequalities. By a limit argument this procedure can define a sort of distinguished self-adjoint extension also when $\nu = 1$ but, in that case, the domain of this self-adjoint extension will be neither contained in the domain of the kinetic energy form nor in the domain of the potential energy form. In a subsequent work, Arrizabalaga [3] weakened further the hypothesis on the construction of the self-adjoint extension of Esteban and Loss.

4 Classification of the Self-Adjoint Extensions

In the previous section we discussed the distinguished extension of the minimal Dirac-Coulomb operator with respect to an infinite multiplicity of others. We come now to the major problem of classifying the one-parameter family of self-adjoint extensions of such an operator.

There is essentially one work, by Hogreve [11], that deals systematically with this problem. There the classification is made by means of von Neumann's extension theory. We start by recalling von Neumann's theorem on general parametrization of symmetric extension.

Theorem 9 (von Neumann) *Let T be a densely defined, closed and symmetric operator. The closed symmetric extensions of T are in one to one correspondence with the set of partial isometries (in the usual inner product) of* $\ker(T^* + i)$ *into* $\ker(T^* - i)$. *If U is such an isometry with initial space $I(U) \subseteq \ker(T^* + i)$, then the corresponding closed symmetric extension T_U has domain*

$$D(T_U) = \{\varphi + \varphi^{(i)} + U\varphi^{(i)} \mid \varphi \in D(T),\ \varphi^{(i)} \in I(U)\} \tag{48}$$

and

$$T_U(\varphi + \varphi^{(i)} + U\varphi^{(i)}) = T\varphi + i\varphi^{(i)} - iU\varphi^{(i)}. \tag{49}$$

If $\dim I(U) < \infty$, *the deficiency indices of T_U are*

$$n_\pm(T_U) = n_\pm(T) - \dim[I(U)]. \tag{50}$$

Recalling that if $\nu^2 > \kappa_j^2 - \frac{1}{4}$ the deficiency indices of t_{m_j,κ_j} are $(1, 1)$, the isometries are just phases: given $\theta \in [0, 2\pi)$ we have

$$\begin{aligned} U_\theta : \ker(T^* + i) &\to \ker(T^* - i) \\ \psi^{(i)} &\mapsto e^{i\theta}\psi^{(-i)}, \end{aligned} \tag{51}$$

and hence at every value of θ there corresponds one self-adjoint extension of the minimal operator t_{m_j,κ_j}.

Let $\psi(r) = (\psi_1(r), \psi_2(r)) \in AC((0,\infty), \mathbb{C}^2)$. We define

$$(\Theta_\theta \psi)(r) = (\psi_2^{(-i)}(r) + e^{i\theta}\psi_2^{(i)}(r), -\psi_1^{(-i)}(r) - e^{i\theta}\psi_1^{(i)}(r)) \cdot \begin{pmatrix} \psi_1(r) \\ \psi_2(r) \end{pmatrix}. \tag{52}$$

Theorem 10 ([11], Theorem 7.1) *Let $|\nu| > \sqrt{\kappa_j^2 - \frac{1}{4}}$, the self-adjoint extensions $t^\theta_{m_j,\kappa_j}$ of the minimal operator t_{m_j,κ_j} of (19) are uniquely determined by $\theta \in [0, 2\pi)$ via the formulas*

$$\mathscr{D}(t^\theta_{m_j,\kappa_j}) = \{\psi \in L^2((0,\infty), \mathbb{C}^2) \cap AC((0,\infty), \mathbb{C}^2) \mid \lim_{r\to 0}(\Theta_\theta \psi)(r), \; t_{m_j,\kappa_j}\psi \in L^2((0,\infty))\} \tag{53}$$

$$t^\theta_{m_j,\kappa_j}\psi = t^*_{m_j,\kappa_j}\psi. \tag{54}$$

Proof We prove only one direction of the theorem.

By von Neumann's theorem above and the explicit formula for the unitary transformation we have

$$\mathscr{D}(t^\theta_{m_j,\kappa_j}) = \mathscr{D}\left(\overline{t^\theta_{m_j,\kappa_j}}\right) + \{c(\psi^{(i)} + e^{i\theta}\psi^{(-i)}) \mid c \in \mathbb{C}\} \tag{55}$$

and hence by taking the limit $r \to 0$ one gets

$$c = \lim_{r\to 0} \frac{\psi_n(r) - \phi_n(r)}{\psi_n^{(-i)} + e^{i\theta}\psi_n^{(i)}(r)} \tag{56}$$

with $n = 1, 2$. This implies that taking into account that $\psi_n \to 0$, for $r \to 0$ the quantity with $n = 1$ equals the one with $n = 2$ and this is precisely the condition $\lim_{r\to 0}(\Theta_\theta \psi) = 0$.

5 Future Perspectives: A Selection of Main Open Problems

In the final part of these notes we survey a few topical questions concerning the multiplicity of self-adjoint realisations of the model.

(i) *Characterisation of $\mathscr{D}(t^\theta_{m_j,\kappa_j})$.* The sole characterisation of the domains of the self-adjoint extensions present in the literature, namely (53) above, does not give any explicit detail on the behaviour of the functions near the origin. More refined information on this short scale behaviour is expected to be achievable by means of the self-adjoint extension theory of Kreĭn-Višik-Birman (KVB) (see for example [16]).

(ii) *Adaptation of the original extension formulas* for initial operators that are not semi-bounded (as is the case for $t^{\theta}_{m_j,\kappa_j}$). The original KVB theory is developed in order to classify the self-adjoint extensions of a semi-bounded operator. An operator version of the extension formula for non semi-bounded operators with a spectral gap can be found in [8, 9] but, to our knowledge, a similar theorem for the corresponding quadratic forms is not available in the literature.

(iii) *Qualification of further features of the domain of the distinguished extension*. Beside the huge amount of studies concerning the domain of the distinguished extension (see for example [3, 4]), the available knowledge on such operator remains somewhat implicit. Among the other informations, one would like to qualify the most singular behaviour at zero of the generic element of the domain, and how this behaviour may depend on the magnitude of the coupling constant ν.

(iv) *General classification of the extensions both in the operator sense and in the quadratic form sense*, where the effectiveness of the classification relies in the possibility of qualifying special subclasses of interest (e.g. invertible ones). In particular, it would be of relevance to reproduce, in analogy to what happens for semi-bounded operators, the natural ordering of the quadratic forms.

(v) *Study of the spectral properties of the generic extension*, with particular focus on the discrete spectrum lying in $[-1, 1]$. For example, one would like to identify the self-adjoint realisation with the highest number of eigenvalues or the one with the lowest eigenvalue or one could even try to identify the lowest possible (absolute value of the) eigenvalue among the extensions.

(vi) *Identification of an analogous notion of distinguished extension in the regime* $\nu > 1$. The reason for which if $\nu > 1$ there is no self-adjoint realisation with the property that its domain is contained in the domain of the potential energy form can be seen with the decomposition (17). If $\nu > 1$ the functions in the domain of the reduced operator in the sector with $j = \frac{1}{2}$ do not vanish at $r = 0$. In all the other sectors, however, this is not the case. It is thus possible to prove the existence of a special self-adjoint realisation of the reduced Dirac operator in the sectors with $j \geq \frac{3}{2}$ that retains most of the properties of the distinguished extension in the regime $\nu \in [\frac{\sqrt{3}}{2}, 1)$.

Acknowledgements This work is partially supported by INdAM (GNFM) and by the 2014–2017 MIUR-FIR grant *Cond-Math: Condensed Matter and Mathematical Physics* code RBFR13WAET.

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Dispersive Estimates for Schrödinger Operators with Point Interactions in $\mathbb{R}^3$

Felice Iandoli and Raffaele Scandone

Abstract The study of dispersive properties of Schrödinger operators with point interactions is a fundamental tool for understanding the behavior of many body quantum systems interacting with very short range potential, whose dynamics can be approximated by non linear Schrödinger equations with singular interactions. In this work we proved that, in the case of one point interaction in $\mathbb{R}^3$, the perturbed Laplacian satisfies the same $L^p - L^q$ estimates of the free Laplacian in the smaller regime $q \in [2, 3)$. These estimates are implied by a recent result concerning the L^p boundedness of the wave operators for the perturbed Laplacian. Our approach, however, is more direct and relatively simple, and could potentially be useful to prove optimal weighted estimates also in the regime $q \geq 3$.

Keywords Dispersive estimates • Point interactions • Schrödinger operators • Weighted Fourier inequalities

1 Introduction

In quantum mechanics, a huge variety of phenomena are described by system of quantum particles interacting with a very short range potentials, supported near away a discrete set of points in $\mathbb{R}^d$. This leads to the study of Hamiltonians which formally are defined as

$$H_{\mu,Y} = \text{“} - \Delta + \sum_{y \in Y} \mu_j \delta_y \text{”} \tag{1}$$

where $-\Delta$ is the free Laplacian on $\mathbb{R}^d$, $Y := \{y_1, y_2, \ldots\}$ is a countable discrete subset of $\mathbb{R}^d$ and μ_{y_j} are real coupling constants. Thus H describes the motion of a quantum particle interacting with a “contact potentials”, created by point sources of strength μ_{y_j} centered at y_j. The first appearance of such Hamiltonians dates back to the celebrated paper of Kronig and Penney [14], where they consider the case

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A. Michelangeli, G. Dell'Antonio (eds.), *Advances in Quantum Mechanics*,
Springer INdAM Series 18, DOI 10.1007/978-3-319-58904-6_11

$d = 1$, $Y = \mathbb{Z}$ and μ_y independent on y as a model of a nonrelativistic electron moving in a fixed crystal lattice. The mathematical rigorous study of $H_{\mu,Y}$ was initiated by Albeverio et al. [1], and subsequently continued by other authors (see for instance [8, 11, 12, 21]). In this work we focus on the case of finitely many point interactions on $\mathbb{R}^3$. The rigorous definition of $H_{\mu,Y}$ is based on the theory of self adjoint extensions of symmetric operators (see [2] for a complete and detailed discussion): one starts with

$$\tilde{H}_Y := -\Delta|\mathscr{C}_0^\infty(\mathbb{R}^3\backslash\{Y\}), \tag{2}$$

which is a densely defined, non-negative, symmetric operator on $L^2(\mathbb{R}^3)$, with deficiency indices (N, N), and hence it admits a N^2-parameter family of self adjoint extensions. Among these, we find the important subfamily of the so called local extensions, characterized by the following proposition (see [2, 9]):

Proposition 1 *Fix* $Y := (y_1, \dots, y_N) \subset \mathbb{R}^3$ *and* $\alpha := (\alpha_1, \alpha_2, \dots, \alpha_N) \in (-\infty, +\infty]^N$. *Given* $z \in \mathbb{C}$, *define*

$$G_z(x) := \frac{e^{iz|x|}}{4\pi|x|}, \qquad \tilde{G}_z(x) := \begin{cases} \frac{e^{iz|x|}}{4\pi|x|} & x \neq 0 \\ 0 & x = 0 \end{cases} \tag{3}$$

and the $N \times N$ *matrix*

$$[\Gamma_{\alpha,Y}(z)]_{(j,l)} := \left[\left(\alpha_j - \frac{iz}{4\pi}\right)\delta_{j,l} - \tilde{G}_z(y_j - y_l)\right]_{(j,l)} \tag{4}$$

The mesomorphic function $z \mapsto [\Gamma_{\alpha,Y}(z)]^{-1}$ *has at most N poles in the upper half space* $\mathbb{C}^+$, *which are all located along the positive imaginary semi-axis. We denote by* $\mathscr{E}$ *the set of such poles. There exists a self adjoint extension* $H_{\alpha,Y}$ *of* $\tilde{H}_Y$ *with the following properties:*

- *Given* $z \in \mathbb{C}^+\backslash\{\mathscr{E}\}$, *the domain of* $H_{\alpha,Y}$ *can be written as:*

$$\mathscr{D}(H_{\alpha,Y}) = \left\{\psi := \phi_z + \sum_{j,l=1}^{N} (\Gamma_{\alpha,Y}(z)^{-1})_{j,l}\phi_z(j_l)G_z(\cdot - y_j)\, ,\ \phi_z \in H^2\right\}. \tag{5}$$

  The decomposition is unique for a given z.
- *With respect to the decomposition* (5), *the action of* $H_{\alpha,Y}$ *is given by*

$$(H_{\alpha,Y} - z^2)\psi := (-\Delta - z^2)\phi. \tag{6}$$

Remark 1 The family of self adjoint operators $H_{\alpha,Y}$ realizes in a rigorous way the heuristic definition given by expression (1). It is worth noticing the different roles played by parameters: while μ_j measures the strength of the point interactions at y_j, α_j is related to the scattering length. Indeed, a generic function $\psi \in \mathscr{D}(H_{\alpha,Y})$

satisfies the so called *Bethe-Peierls contact condition*

$$\psi(x) \underset{x \to y_i}{\sim} \frac{1}{|x - y_j|} + 4\pi\alpha_j, \quad j = 1, \ldots, N \tag{7}$$

which is typical for the low-energy behavior of an eigenstate of the Schrödinger equation for a quantum particle subject to a very short range potential, centered at y_j and with s-wave scattering length $-(4\pi\alpha_j)^{-1}$ (see the works of Bethe and Peierls [5, 6]). When $\alpha_j = +\infty$, no actual interactions take place at y_j (the s-wave has zero scattering length); in particular when $\alpha = +\infty$ we recover the Friedrichs extension of $\tilde{H}_Y$, namely the free Laplacian on $L^2(\mathbb{R}^3)$.
The spectral properties of $H_{\alpha,Y}$ are well known and completely characterized; we encode them in the following proposition (see [2, 9]):

Proposition 2

1. *The spectrum $\sigma(H_{\alpha,Y})$ of $H_{\alpha,Y}$ consists of at most N negative eigenvalues and the absolutely continuous part $\sigma_{ac}(H_{\alpha,Y}) = [0, +\infty)$. Moreover, there exists a one to one correspondence between the poles $i\lambda \in \mathscr{E}$ and the negative eigenvalues $-\lambda^2$ of $H_{\alpha,Y}$, counted with multiplicity.*
2. *The resolvent of $H_{\alpha,Y}$ is a rank N perturbation of the free resolvent, and it is given by:*

$$(H_{\alpha,Y} - z^2)^{-1} - (H_0 - z^2)^{-1} \;=\; \sum_{j,k=1}^{N} (\Gamma_{\alpha,Y}(z)^{-1})_{jk}\, G_z^{y_j} \otimes \overline{G_z^{y_k}}. \tag{8}$$

We conclude this introduction by observing that $H_{\alpha,Y}$ can be also realized as limit of scaled short range Schrödinger operator. Indeed we have the following Proposition (see [2]):

Proposition 3 *Fix $\alpha \in (-\infty, +\infty]^N$ and $Y = \{y_1, \ldots, y_N\} \subset \mathbb{R}^3$. There exist real valued potentials $V_1, \ldots V_N$ of finite Rollnik norm, and real analytic functions $\lambda_j : \mathbb{R} \to \mathbb{R}$, with $\lambda_j(0) = 1$, such that the family of Schrödinger operators*

$$H_\varepsilon := -\Delta + \sum_{j=1}^{N} \frac{\lambda_j(\varepsilon)}{\varepsilon^2} V\left(\frac{x - y_j}{\varepsilon}\right) \tag{9}$$

converges in strong resolvent sense to $H_{\alpha,Y}$ as ε goes to zero. Moreover:

$$\alpha_j \neq +\infty \text{ for some } j \iff -\Delta + V_j \text{ has a zero energy resonance.} \tag{10}$$

Remark 2 Proposition 3 makes more convincing the idea of considering the Hamiltonian $H_{\alpha,Y}$ as an approximation of more realistic phenomena, governed by very short range interactions.

2 Dispersive Properties of $H_{\alpha,Y}$

Since H_α is a self adjoint operator, it generates a unitary group of operators $e^{itH_{\alpha,Y}}$; in particular the L^2 norm is preserved by the evolution:

$$\|e^{itH_{\alpha,Y}}f\|_{L^2(\mathbb{R}^3)} = \|f\|_{L^2(\mathbb{R}^3)}. \tag{11}$$

It is natural to investigate the dispersive properties of $e^{itH_{\alpha,Y}}$. The first work in this direction is by D'ancona et al. [7], who proved weighted $L^1 - L^\infty$ estimates

$$\|w^{-1}e^{itH_{\alpha,Y}}P_{ac}f\|_{L^\infty(\mathbb{R}^3)} \lesssim t^{-\frac{3}{2}}\|wf\|_{L^1(\mathbb{R}^3)} \tag{12}$$

where P_{ac} is the projection onto the absolutely continuous spectrum of $H_{\alpha,Y}$ and

$$w(x) = \sum_{j=1}^{N}\left(1 + \frac{1}{|x-y_j|}\right), \tag{13}$$

under the following assumption:

Assumption 1 *The matrix $\Gamma_{\alpha,Y}(z)$ is invertible for $z \geq 0$, with locally bounded inverse.*

It is worth noticing that the presence of a weight in (12) is unavoidable, because of the singularities appearing in the domain of $H_{\alpha,Y}$. In the case of one single point interaction, Assumption 1 is always satisfied except for $\alpha = 0$, in which case the perturbed Hamiltonian has a zero energy resonance. Nevertheless, exploiting the explicit formula for the propagator e^{itH} available in the case $N = 1$ (see [3, 18]), also the case $\alpha = 0$ was settle down in [7], by showing weighted dispersive inequality with a slower decay in t, a typical phenomenon for Schrödinger operators with zero energy resonances:

$$\|w^{-1}e^{itH_{0,y}}f\|_{L^\infty(\mathbb{R}^3)} \lesssim t^{-\frac{1}{2}}\|wf\|_{L^1(\mathbb{R}^3)}. \tag{14}$$

Observe now that, interpolating (12) and (14) with the trivial bound (11), we get weighted dispersive inequalities in the full range $q \in [2, +\infty]$:

Proposition 4

1. *Under Assumption 1, the following estimates holds:*

$$\|w^{-\left(1-\frac{2}{q}\right)}e^{itH_{\alpha,Y}}P_{ac}f\|_{L^q(\mathbb{R}^3)} \lesssim t^{-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{q}\right)}\|w^{\frac{2}{p}-1}f\|_{L^p(\mathbb{R}^3)} \tag{15}$$

where $q \in [2, +\infty]$ and p is the dual exponent of q.

2. *In the case $N = 1$, $\alpha = 0$ we have*

$$\|w^{-\left(1-\frac{2}{q}\right)} e^{itH_{0,y}} f\|_{L^q(\mathbb{R}^3)} \lesssim t^{-\frac{1}{2}\left(\frac{1}{p}-\frac{1}{q}\right)} \|w^{\frac{2}{p}-1} f\|_{L^p(\mathbb{R}^3)} \tag{16}$$

where $q \in [2, +\infty]$ and p is the dual exponent of q.

However, since the singularities $G_i(x - y_j)$ belong to $L^q(\mathbb{R}^3)$ for $q \in [2, 3)$, one may hope, at least in principle, to prove an unweighted version of (15) and (16). This is true indeed, and it is a consequence of a recent result [9]:

Theorem 1 *For any Y and α, the wave operators*

$$W^{\pm}_{\alpha,Y} = s - \lim_{t\to+\infty} e^{itH_{\alpha,Y}} e^{it\Delta} \tag{17}$$

for the pair $(H_{\alpha,Y}, -\Delta)$ exist and are complete on $L^2(\mathbb{R}^3)$, and they are bounded on $L^q(\mathbb{R}^3)$ for $1 < q < 3$.

Remark 3 The restriction $1 < q < 3$ already emerges at level of approximating Schrödinger operators. Indeed, if $H = -\Delta + V$ has a zero energy resonance (which by Proposition 3 is a necessary condition for H_ε to converges to H), then the wave operators

$$W^{\pm}_{V} := s - \lim_{t\to+\infty} e^{it(-\Delta+V)} e^{it\Delta} \tag{18}$$

are bounded on L^q if and only if $1 < q < 3$ (see Yajima [20])
Owing to Theorem 1 and the intertwining property of wave operators, viz.

$$f(H_{\alpha,Y}) P_{ac} H_{\alpha,Y} = W^{\pm}_{\alpha,Y} f(-\Delta)(W^{\pm}_{\alpha,Y})^* \tag{19}$$

for any Borel function f on $\mathbb{R}^3$, one can lift the classical dispersive estimates for the free Laplacian into analogous estimates for $H_{\alpha,Y}$, albeit for the restriction on the exponent q. Thus we find:

Proposition 5 *For any α and Y, we have the estimate*

$$\|e^{itH_{\alpha,Y}} P_{ac} f\|_{L^q(\mathbb{R}^3)} \lesssim t^{-\frac{3}{2}(\frac{1}{p}-\frac{1}{q})} \|f\|_{L^p(\mathbb{R}^3)} \qquad \text{for } q \in [2, 3). \tag{20}$$

Interpolating (20) respectively with (12) and (14), we deduce also the following:

Corollary 1

1. *Under Assumption 1, we have*

$$\|w^{-\left(1-\frac{3-\varepsilon}{q}\right)} e^{itH_{\alpha,Y}} P_{ac} f\|_{L^q(\mathbb{R}^3)} \lesssim t^{-\frac{3}{2}(\frac{1}{p}-\frac{1}{q})} \|w^{\left(1-\frac{3-\varepsilon}{q}\right)} f\|_{L^p(\mathbb{R}^3)} \tag{21}$$

in the regime $q \in [3, +\infty]$.

2. *When* $N = 1$ *and* $\alpha = 0$, *we have*

$$\|w^{-\left(1-\frac{3-\varepsilon}{q}\right)} e^{itH_{0,y}} f\|_{L^q(\mathbb{R}^3)} \lesssim t^{-\frac{1}{2}+\frac{\varepsilon}{q}} \|w^{\left(1-\frac{3-\varepsilon}{q}\right)} f\|_{L^p(\mathbb{R}^3)} \tag{22}$$

in the regime $q \in [3, +\infty]$.

We can see that the results in [9] improves the one in [7] in various ways:

1. In the regime $q \in [2, 3)$, with an arbitrary number of centers, both the weights and the hypothesis 1 on Γ are removed.
2. In the regime $q \in [3, +\infty]$, with an arbitrary number of centers and under the hypothesis 1, the weights are strengthened to be almost optimal [indeed we can not remove ε in estimate (21)].
3. In the case $N = 1$, $\alpha = 0$ and in the regime $q \in [2, 3)$, the weights are removed and the time decay is strengthened.
4. In the case $N = 1$, $\alpha = 0$ and in the regime $q \in [3, +\infty]$, both the weights and the time decay are strengthened, and again the weights are almost optimal.

In this work we want to provide a new and simpler proof of Proposition 5 in the particular case $N = 1$, without using any knowledge about the wave operators.

3 Proof of Proposition 5, Case $N = 1$

The operators H_{α,y_1} and H_{α,y_2} are conjugated by translations, hence we can assume $y = 0$ and we will simply write H_α instead of $H_{\alpha,0}$. We recall an useful factorization for the operator H_α (see [2]). Introducing spherical coordinates on $\mathbb{R}^3$, we can decompose $L^2(\mathbb{R}^3)$ with respect to angular momenta:

$$L^2(\mathbb{R}^3) = L^2(\mathbb{R}^+, r^2 dr) \otimes L^2(S^2) \tag{23}$$

where S^2 is the unit sphere in $\mathbb{R}^3$. Moreover, using the unitary transformation

$$U : L^2((0, +\infty), r^2 dr) \to L^2(\mathbb{R}^+, r dr), \quad (Uf)(r) = rf(r) \tag{24}$$

and decomposing $L^2(S^2)$ into spherical harmonics

$$\{Y_{l,m} l \in \mathbb{N}, m = 0, \pm 1, \ldots, \pm l\}\,, \tag{25}$$

we obtain

$$L^2(\mathbb{R}^3) = \bigoplus_{l=0}^{+\infty} U^{-1} L^2(\mathbb{R}^+, rdr) \otimes \langle Y_{l,-l}, \ldots, Y_{l,l}\rangle. \tag{26}$$

With respect to this decomposition, the symmetric operator $\tilde{H} := \tilde{H}_{\{0\}}$ writes as

$$\tilde{H} = \bigoplus_{l=0}^{+\infty} U^{-1} h_l U \otimes 1 \tag{27}$$

where h_l, $l \geq 0$ are symmetric operators on $L^2(\mathbb{R}^+)$, with common domain $\mathscr{C}_0^\infty(\mathbb{R}^+)$ and actions given by

$$h_l = -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2}, \quad r > 0. \tag{28}$$

It is well known [17] that h_l are essentially self adjoint for $l \geq 1$, while h_0 admits a one parameter family of selfadjoint extension $\dot{h}_{0,\alpha}$ such that

$$H_\alpha = \dot{h}_{0,\alpha} \oplus \bigoplus_{l=1}^{+\infty} U^{-1} \dot{h}_l U \otimes 1 \tag{29}$$

where $\dot{h}_l$ is the unique self adjoint extension of h_l, for $l \geq 1$. Identity (29) tells us that H_α completely diagonalizes with respect to decomposition (26), and that it coincides with $-\Delta$ after projecting out the subspace of radial functions. Hence it immediately follows

Lemma 1 *Suppose $f \in L^2(\mathbb{R}^3)$ is orthogonal to the subspace of radial functions. Then*

$$e^{itH_\alpha} f = e^{-it\Delta} f \tag{30}$$

Lemma 1 has an important Corollary, which considerably simplifies our proof:

Corollary 2 *In the proof of Proposition 5 (in the special case $N = 1$) we can suppose f to be radial.*

Proof Suppose (20) to be true for radial functions. Given a generic $f \in L^2(\mathbb{R}^3)$, we can decompose it as $f_1 + f_2$, where

$$f_1 := \frac{4\pi}{|y|^2} \int_{S_y} f(r,\omega) d\mathscr{H}^2(\omega) \tag{31}$$

is the orthogonal projection onto $L^2_{rad}(\mathbb{R}^3)$. By Lemma 1, we get

$$e^{itH_\alpha} f = e^{itH_\alpha} f_1 + e^{-it\Delta} f_2. \tag{32}$$

By hypothesis and using the dispersive estimates for the free Laplacian, we deduce

$$\|e^{itH_\alpha} f\|_{L^q} \le t^{\frac{3}{2}\left(\frac{1}{p}-\frac{1}{q}\right)}(\|f_1\|_{L^p} + \|f_2\|_{L^p}). \tag{33}$$

Now, using Hölder inequality, we get

$$\begin{aligned}\|f_1\|_{L^p}^p &\le \int_0^{+\infty} r^{2-2p}\left(\int_{S_r} |f(r,\omega)| d\mathscr{H}^2(\omega)\right)^p dr \\ &\le \int_0^{+\infty} r^{2-2p+\frac{2p}{q}} \int_{S_r} |f(r,\omega)|^p d\mathscr{H}^2(\omega) dr = \\ &\int_0^{+\infty}\int_{S_r} ||f(r,\omega)| d\mathscr{H}^2(\omega)|^p = \|f\|_{L^p}^p\end{aligned}$$

and consequently

$$\|f_2\|_{L^p} \le \|f\|_{L^p} + \|f_1\|_{L^p} \lesssim \|f\|_{L^p} \tag{34}$$

which concludes the proof.

Now we are in turn to prove our main result. As mentioned before, in the case $N = 1$, the propagator associated to H_α is explicitly known. In particular, Scarlatti and Teta [18] have proved the following characterization:

$$e^{itH_\alpha} f = \begin{cases} e^{-it\Delta} f + \lim_{R\to\infty} M_R f & \text{if } \alpha = 0 \\ e^{itH_0} f + \lim_{R\to\infty} M_{\alpha,R} f & \text{if } \alpha > 0 \\ e^{itH_0} f + \lim_{R\to\infty} \widetilde{M}_{\alpha,R} f & \text{if } \alpha < 0 \end{cases} \tag{35}$$

where the limit is taken in the L^2 sense and

$$M_R f(x) := (4\pi it)^{-1/2} \frac{1}{4\pi|x|} \int_{B_R} \frac{\widetilde{f}(|y|)}{|y|} e^{-i\frac{(|x|+|y|)^2}{4t}} dy, \tag{36}$$

$$M_{\alpha,R} f(x) := -(4\pi it)^{-1/2} \frac{\alpha}{|x|} \int_{\mathbb{R}^3} \frac{f(y)}{|y|} \int_0^{+\infty} e^{-4\pi\alpha s} e^{-i\frac{(|x|+|y|+s)^2}{4t}} ds dy, \tag{37}$$

$$\begin{aligned}\widetilde{M}_{\alpha,R} f(x) := \Bigg(&-\psi_\alpha(x)\int_{B_R} \psi_\alpha(y) f(y) e^{it(4\pi\alpha)^2} dy \\ &- \frac{\alpha}{|x|}(it\pi)^{-1/2} \int_{B_R} \frac{f(y)}{|y|} \int_0^{+\infty} e^{4\pi\alpha s} \exp\left(-\frac{(u-|x|-|y|)^2}{4it}\right) ds dy\Bigg),\end{aligned} \tag{38}$$

and $\psi_\alpha(x) = \sqrt{-2\alpha}\frac{e^{4\pi\alpha|x|}}{|x|}$ is the normalized eigenfunction associated to the negative eigenvalue $-(4\pi\alpha)^2$ for $\alpha < 0$. We are going to show that the following estimates hold uniformly in $R > 0$:

$$\|M_R f\|_{L^q} \lesssim t^{-\frac{3}{2}(\frac{1}{p}-\frac{1}{q})}\|f\|_{L^p}, \tag{39}$$

$$\|M_{\alpha,R} f\|_{L^q} \lesssim t^{-\frac{3}{2}(\frac{1}{p}-\frac{1}{q})}\|f\|_{L^p}, \tag{40}$$

$$\|\widetilde{M}_{\alpha,R} P_{ac} f\|_{L^q} \lesssim t^{-\frac{3}{2}(\frac{1}{p}-\frac{1}{q})}\|f\|_{L^p}. \tag{41}$$

The latter inequalities are clearly sufficient to prove Proposition 5 in the special case $N = 1$. Let us start by proving inequality (39). Thanks to Corollary 2 we can suppose $f(y) = \widetilde{f}(|y|)$ for some $\widetilde{f} : \mathbb{R} \to \mathbb{R}$. Using spherical coordinates in both variables x and y we get

$$\|M_R f\|_{L^q} \lesssim t^{-1/2}\left[\int_0^{+\infty} r^{2-q}\left|\int_0^R \exp\left(-i\frac{\rho r}{2t} - i\frac{\rho^2}{4t}\right)\rho\widetilde{f}(\rho)d\rho\right|^q dr\right]^{1/q}. \tag{42}$$

Setting

$$h(\rho) := \begin{cases} e^{-i\rho^2/4t}\rho\widetilde{f}(\rho) & 0 \le \rho \le R \\ 0 & \rho \in \mathbb{R}\setminus[0,R] \end{cases} \tag{43}$$

the latter expression becomes

$$t^{-1/2}\left[\int_0^{+\infty} r^{2-q}\left|\widehat{h}\left(\frac{r}{2t}\right)\right|^q dr\right]^{1/q}, \tag{44}$$

which is equal to

$$t^{-\frac{3}{2}(\frac{1}{p}-\frac{1}{q})}\left[\int_0^{+\infty} r^{2-q}|\widehat{h}(r)|^q dr\right]^{1/q}. \tag{45}$$

At this point we are ready to use a classical weighted Fourier transform norm inequality, also known in literature as Pitt's inequality. We state here the original theorem proved by Pitt in 1937 [16]:

Theorem 2 (Pitt's Theorem) *Let* $1 < \gamma \le \eta < \infty$, *choose* $0 < b < \frac{1}{\gamma'}$ *with* $\frac{1}{\gamma} + \frac{1}{\gamma'} = 1$, *set* $\beta = 1 - \frac{1}{\gamma} - \frac{1}{\eta} - b < 0$ *and define* $v(x) = |x|^{b\gamma}$ *for all* $x \in \mathbb{R}$. *There is a constant* $C > 0$ *such that*

$$\left(\int_{\mathbb{R}} |\widehat{f}(\xi)|^\eta |\xi|^{\beta\eta} d\xi\right)^{1/\eta} \le C\left(\int_{\mathbb{R}} |f(x)|^\gamma |x|^{b\gamma} dx\right)^{1/\gamma}, \tag{46}$$

for all $f \in L^\gamma_v(\mathbb{R})$.

Since $q < 3$ we may use this Theorem in the case $\eta = q$, $\gamma = p$, $\beta = \frac{2-q}{q}$ and $b = \frac{2-p}{p}$ obtaining

$$t^{-\frac{3}{2}(\frac{1}{p}-\frac{1}{q})}\left[\int_0^{+\infty} r^{2-q}|\widehat{h}(r)|^q dr\right]^{1/q} \lesssim t^{-\frac{3}{2}(\frac{1}{p}-\frac{1}{q})}\left[\int_0^{+\infty} |h(r)|^p r^{2-p} dr\right]^{1/p}, \tag{47}$$

which essentially is the desired estimate, indeed

$$\left[\int_0^{+\infty} |h(r)|^p r^{2-p} dr\right]^{1/p} = \|f\|_{L^p}. \tag{48}$$

This concludes the proof of (39), which, together with the standard dispersive estimates for the free Laplacian, implies the dispersive estimates for the semigroup $\{e^{itH_0}\}_{t>0}$.

Let us turn in to proving (40). Since $q < 3$ the function $1/|y|$ belongs to $L^q(B_R)$, hence we can exchange the order of integration and use Minkowski inequality

$$\begin{aligned}
&\|M_R f\|_{L^q} \lesssim \\
&\lesssim t^{-1/2}\int_0^{+\infty}\left\|\int_{B_R}\frac{1}{|x|}\exp\left(-4\pi\alpha s - i\frac{(|x|+|y|+s)^2}{4t}\right)\frac{\widetilde{f}(y)}{|y|}dy\right\|_{L^q} ds \\
&= t^{-1/2}\int_0^{+\infty} e^{-4\pi\alpha s}\left\|\int_{B_R}\frac{1}{|x|}\exp\left(-i\frac{|y|^2}{4t} - i\frac{|x||y|}{2t} - i\frac{s|y|}{2t}\right)\frac{f(y)}{|y|}dy\right\|_{L^q} ds,
\end{aligned} \tag{49}$$

which, as before, in spherical coordinates is bounded, up to constants, by

$$t^{-1/2}\int_0^{+\infty} e^{-4\pi\alpha s}\left(\int_0^{+\infty} r^{2-q}\left|\int_0^R e^{-i\frac{r\rho}{2t}} h_s(\rho)(\rho)d\rho\right|^q dr\right) ds, \tag{50}$$

where

$$h_s(\rho) := \begin{cases} \exp\left(-i\frac{\rho^2}{4t} - i\frac{s\rho}{2t}\right)\rho\widetilde{f}(\rho) & 0 \le \rho \le R \\ 0 & \rho \in \mathbb{R}\setminus[0,R] \end{cases}. \tag{51}$$

The quantity (50) is nothing but

$$t^{-1/2}\int_0^{+\infty} e^{-4\pi\alpha s}\left(\int_0^{+\infty} r^{2-q}\left|\widehat{h_s}\left(\frac{r}{2t}\right)\right|^q dr\right)^{1/q} ds, \tag{52}$$

which, arguing as before, is bounded by $t^{-\frac{3}{2}(\frac{1}{p}-\frac{1}{q})}\|f\|_{L^p}$. This concludes the proof of (40).

The proof of (41) is very similar, indeed after projecting f onto the absolutely continuous spectrum of H_α, the first summand in the right hand side of (38) disappears and hence the remaining part can be treated exactly in the same way as done in the proof of (40).

4 Conclusions

The proof given in Sect. 3 is quite direct and does not use any deep results from scattering theory for the perturbed Hamiltonian $H_{\alpha,Y}$. Nevertheless, it is worth noticing that the proof of Pitt's inequality, the main tool of our argument, requires some technical results from harmonic analysis such as Muckenhaupt estimates [10, 15], which play an essential role also in the proof of the L^p boundedness of the wave operators $W^\pm$ given in [9]. The main advantage of our approach is that, owing to more general weighted Fourier inequalities (see for instance [4, 13]) rather than Pitt's inequality (in which the weights are forced to be pure powers), it can potentially be adapted to prove optimal $L^p - L^q$ estimates also in the regime $q \geq 3$. In particular, we conjecture the following result:

Conjecture 1 Fix $q \in [3, +\infty]$, and let $w_q(x)$ a weight such that $w(x) \equiv 1$ outside a ball centered at the origin and $w_q^{-1} G_i \in L^q(\mathbb{R}^3)$. Then for every $\alpha \neq 0$ and $y \in \mathbb{R}^3$, the following estimates hold:

$$\|w_q(\cdot - y)^{-1} e^{itH_{\alpha,y}} P_{ac} f\|_{L^q(\mathbb{R}^3)} \lesssim t^{-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{q}\right)} \|w_q(\cdot - y) f\|_{L^p(\mathbb{R}^3)}. \tag{53}$$

When $\alpha = 0$, a similar estimate holds but with a slower time decay:

$$\|w_q(\cdot - y)^{-1} e^{itH_{\alpha,y}} f\|_{L^q(\mathbb{R}^3)} \lesssim t^{-\frac{1}{2}} \|w_q(\cdot - y) f\|_{L^p(\mathbb{R}^3)}. \tag{54}$$

Remark 4 Conjecture 1 is motivated by the natural principle for which removing the local singularity is enough to get dispersive estimates, and it would improve the result in Corollary 1. For example when $q = 3$ we expect that a logarithmic weight would suffice, while in estimates (21) and (22) there appear polynomial weights.
An alternative conjecture can be expressed in term of weighted Lorentz space, in which context there are other generalizations of Pitt's inequality (see for instance [19]):

Conjecture 2 Given $q \in [3, +\infty]$, define the weight

$$w_q := 1 + |x|^{\frac{3}{q}-1}$$

Then for every $\alpha \neq 0$ and $y \in \mathbb{R}^3$, the following estimates hold:

$$\left\| w_q(\cdot - y)^{-1} e^{itH_{\alpha,y}} P_{ac} f \right\|_{L^{q,\infty}(\mathbb{R}^3)} \lesssim t^{-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{q}\right)} \left\| w_q(\cdot - y) f \right\|_{L^{p,1}(\mathbb{R}^3)} . \tag{55}$$

When $\alpha = 0$, a similar estimates holds but with a slower time decay:

$$\left\| w_q(\cdot - y)^{-1} e^{itH_{\alpha,y}} f \right\|_{L^{q,\infty}(\mathbb{R}^3)} \lesssim t^{-\frac{1}{2}} \left\| w_q(\cdot - y) f \right\|_{L^{p,1}(\mathbb{R}^3)} . \tag{56}$$

Remark 5 The function $w_q^{-1} G_i$ belongs to $L^{q,\infty}(\mathbb{R}^3)$, hence the plausibility of the conjecture. Observe moreover that it would be enough to prove (55) and (56) when $q = 3$, the general case following by interpolation with $q = \infty$, in which case we recover the weighted $L^1 - L^\infty$ estimates (12) and (14) proved in [7].

Acknowledgements Raffaele Scandone is partially supported by the 2014–2017 MIUR-FIR grant "*Cond-Math: Condensed Matter and Mathematical Physics*", code RBFR13WAET and by Gruppo Nazionale per la Fisica Matematica (GNFM-INdAM).

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Chern and Fu–Kane–Mele Invariants as Topological Obstructions

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Abstract The use of topological invariants to describe geometric phases of quantum matter has become an essential tool in modern solid state physics. The first instance of this paradigmatic trend can be traced to the study of the quantum Hall effect, in which the Chern number underlies the quantization of the transverse Hall conductivity. More recently, in the framework of time-reversal symmetric topological insulators and quantum spin Hall systems, a new topological classification has been proposed by Fu, Kane and Mele, where the label takes value in $\mathbb{Z}_2$.

We illustrate how both the Chern number $c \in \mathbb{Z}$ and the Fu–Kane–Mele invariant $\delta \in \mathbb{Z}_2$ of 2-dimensional topological insulators can be characterized as topological obstructions. Indeed, c quantifies the obstruction to the existence of a frame of Bloch states for the crystal which is both continuous and periodic with respect to the crystal momentum. Instead, δ measures the possibility to impose a further time-reversal symmetry constraint on the Bloch frame.

Keywords Chern numbers • Fu–Kane–Mele invariants • Obstruction theory • Quantum hall effect • Quantum spin hall effect • Topological insulators

1 Introduction

One of the most prominent instances of Wigner's "unresonable effectiveness of mathematics" in condensed matter systems is provided by *topological insulators* [15]. These materials, although insulating in the bulk, have the property of conducting currents on their boundary, making them amenable to various types of applications in material science, and even in quantum computing. A thorough understanding of the transport properties of these materials, however, can be achieved only by investigating the topology of the occupied states that fill the bulk energy bands, by virtue of a principle known as the bulk-edge correspondence. Consequently, some of the techniques of topology and differential geometry, once

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A. Michelangeli, G. Dell'Antonio (eds.), *Advances in Quantum Mechanics*,
Springer INdAM Series 18, DOI 10.1007/978-3-319-58904-6_12

relegated to abstract mathematics, have nowadays become common knowledge also among solid state physicists.

To better understand how topology enters in the world of condensed matter systems, it is particularly instructive to consider the archetypal example of a topological insulator, given by a *quantum Hall system* [13]. An effectively 2-dimensional crystalline medium is immersed in a uniform magnetic field perpendicular to the plane of the sample, and an electric current is driven in one direction along the crystal. The induced current is measured in the transverse direction. In a remarkable experiment, performed at very low temperatures by von Klitzing and his collaborators [28], the (Hall) conductivity σ_{H} associated to this transverse current was shown to display *plateaux* which occurred at integer multiples of a fundamental constant, measured moreover with an astounding precision:

$$\sigma_{\mathrm{H}} = n\,\frac{e^2}{h}, \quad n \in \mathbb{Z}. \tag{1}$$

Later theoretical investigations showed that a topological phenomenon underlies this quantization: the integer n in the above formula was shown to be the first Chern number of a vector bundle, naturally associated to the quantum system [1, 2, 27].

The only role played by the magnetic field in quantum Hall systems is that of breaking *time-reversal symmetry*: if the system were time-reversal symmetric, then the Hall conductivity would vanish, and the system would remain in an insulating state. This fact was clarified by Haldane [14], who showed that non-trivial topological phases can be displayed also in absence of a magnetic field, thus initiating the field of *Chern insulators* [3, 5]. Picking up on the work by Haldane, Fu, Kane and Mele [11, 12, 18] later introduced a model which still displays a topological phase even if time-reversal symmetry is preserved, and is by now recognized as a milestone in the history of topological insulators. The phenomenon that the model proposed to illustrate is that of the *quantum spin Hall effect*, which differs from the quantum Hall effect in that the external magnetic field is replaced by spin-orbit interactions (exactly to preserve time-reversal symmetry), and spin rather than charge currents flow on the boundary of the sample. From the point of view of topological phases, the peculiarity of this phenomenon is that, contrary to what happens for Chern and quantum Hall insulators, one can only distinguish between the trivial (insulating) and non-trivial (quantum spin Hall) phase: the label is then assigned by a $\mathbb{Z}_2$-valued topological index. Giving a full account of the geometric nature of this invariant has been a primary objective for mathematical physicists in the last decade, and a plethora of mathematical tools has been used in this endeavour, ranging from K-theory to homotopy theory, from functional analysis to noncommutative geometry, from equivariant cohomology to operator theory. We refer to [7, 10, 25] for recent accounts on the ever-growing literature on the subject.

The purpose of this contribution is to express both the Chern number and the Fu–Kane–Mele $\mathbb{Z}_2$ index of 2-dimensional topological insulators in a common framework, provided by *obstruction theory*. It will be shown how both invariants arise as *topological obstructions* to the existence of a Bloch frame, which roughly speaking can be described as a set of continuous functions which parametrize the occupied states of the physical systems and are compatible with its symmetries, namely periodicity with respect to the Bravais lattice of the crystal and, possibly, time-reversal symmetry; a precise definition will be given in the next Section. The nature of these topological invariants as obstructions was early realized [11, 20], employing methods from bundle theory and using local trivializing charts. Our strategy relies instead on successive extensions of the definition of the Bloch frame, which is well-suited for induction on the dimension of the system and is reminiscent of the extension of a section of a bundle along the cellular decomposition of its base space. We use only basic facts from linear algebra and the topology of the group of unitary matrices $\mathrm{U}(m)$; besides, our method has the further advantage of constructing the required Bloch frame in an algorithmic fashion.

2 Topology of Crystalline Systems

2.1 Periodic Hamiltonians

To set up a rigorous investigation of topological phases of quantum matter, we first have to understand the mathematical description of crystalline systems. The starting point is a *periodic Hamiltonian*: one could think of continuous models described by Schrödinger operators, or of discrete, tight-binding models described by hopping matrices. Periodicity means that the operator H should commute with the translations associated to a lattice $\Gamma \simeq \mathbb{Z}^d \subset \mathbb{R}^d$, namely the Bravais lattice of the crystal under scrutiny. This symmetry of the Hamiltonian leads to a partial diagonalization of it, by looking at common (generalized) eigenstates for the Hamiltonian and the translations: this procedure, which is reminiscent of the Fourier decomposition, goes by the name of *Bloch-Floquet reduction* [22]. In this representation, the Hamiltonian becomes a fibered operator, with fibre $H(k)$ acting on a space $\mathscr{H}_{\mathrm{f}}$ containing the degrees of freedom associated to a unit cell for Γ. The parameter $k \in \mathbb{R}^d$, also called *crystal* or *Bloch momentum*, is determined up to translations by vectors in the dual lattice $\Lambda := \Gamma^*$, and thus can be considered as an element of the *Brillouin torus* $\mathbb{T}^d := \mathbb{R}^d/\Lambda$. Indeed, the fibre Hamiltonians at k and $k+\lambda$, $\lambda \in \Lambda$, are unitarily intertwined by a representation $\tau\colon \Lambda \to \mathscr{U}(\mathscr{H}_{\mathrm{f}})$, namely

$$H(k+\lambda) = \tau_\lambda \, H(k) \, \tau_\lambda^{-1}.$$

The above relation will be called *τ-covariance* in what follows.

Due to the compactness of the unit cell, under fairly general assumptions[1] the operator $H(k)$ has discrete spectrum: the function $k \mapsto E_n(k)$, associated to one of

[1]In continuous models, where H is a Schrödinger operator, these assumptions usually amount to asking that the electromagnetic potentials be infinitesimally Kato-small (possibly in the sense of quadratic forms) with respect to the kinetic part [26].

its eigenvalues (labelled, say, in increasing order), is called the *Bloch band*. The spectrum of the original Hamiltonian is recovered by considering the (possibly overlapping) ranges of all these functions, and leads to the well-known band-gap structure of the spectrum of a periodic operator. If one assumes that the Fermi energy of the system lies in a spectral gap for H, then it makes sense to consider the Fermi projector $P(k)$ on the m occupied bands. The gap condition implies that the dependence of $P(k)$ on k is analytic, and the family of operators $P(k)$ is also τ-covariant (see e.g. [24, Proposition 2.1]).

For the applications to topological insulators that we are aiming at, we need to consider also a further symmetry of the Hamiltonian, namely *time-reversal symmetry*. This is implemented antiunitarily on the Hilbert space of the quantum particle, and flips the arrow of time (and hence the crystal momentum). Mathematically, this amounts to require the existence of an antiunitary operator Θ on $\mathscr{H}_{\mathrm{f}}$, squaring to $\pm\mathbf{1}_{\mathscr{H}_{\mathrm{f}}}$, and such that

$$H(-k) = \Theta\, H(k)\, \Theta^{-1}.$$

We say that the family of operators $H(k)$ is *time-reversal symmetric* if the above holds. It is easy to verify that the Fermi projectors associated to a time-reversal symmetric Hamiltonians are time-reversal symmetric as well. In what follows, we will focus mainly on the case of a *fermionic* time-reversal symmetry operator, namely on the case where $\Theta^2 = -\mathbf{1}_{\mathscr{H}_{\mathrm{f}}}$, as is the case for example for quantum spin Hall systems.

2.2 Bloch Bundle, Berry Connection and Berry Curvature

From the previous analysis of periodic and time-reversal symmetric Hamiltonians, we ended up with a family of projectors $\{P(k)\}_{k\in\mathbb{R}^d} \subset \mathscr{B}(\mathscr{H}_{\mathrm{f}})$, $P(k)^* = P(k) = P(k)^2$, satisfying the following properties:

(P_1) *analyticity*: the map $k \mapsto P(k)$ is a real-analytic map on $\mathbb{R}^d$ with values in $\mathscr{B}(\mathscr{H}_{\mathrm{f}})$;

(P_2) *τ-covariance*: the map $k \mapsto P(k)$ satisfies

$$P(k+\lambda) = \tau_\lambda\, P(k)\, \tau_\lambda^{-1}$$

for a unitary representation $\tau\colon \Lambda \to \mathscr{U}(\mathscr{H}_{\mathrm{f}})$ of the lattice $\Lambda \simeq \mathbb{Z}^d \subset \mathbb{R}^d$;

(P_3) *time-reversal symmetry*: the map $k \mapsto P(k)$ satisfies

$$P(-k) = \Theta\, P(k)\, \Theta^{-1}$$

for an antiunitary operator $\Theta\colon \mathscr{H}_{\mathrm{f}} \to \mathscr{H}_{\mathrm{f}}$ such that $\Theta^2 = -\mathbf{1}_{\mathscr{H}_{\mathrm{f}}}$.

The topology underlying the quantum system described by the Hamiltonian H is encoded in its eigenprojectors, satisfying the above properties.[2] Indeed, one can associate to any family of projectors satisfying (P_1) and (P_2) a vector bundle $\mathscr{E}$ over the torus $\mathbb{T}^d$, called the *Bloch bundle*, via a procedure reminiscent of the Serre–Swan construction: the fibre of $\mathscr{E}$ over the point $k \in \mathbb{T}^d$ is the m-dimensional vector space $\operatorname{Ran} P(k)$ (we refer to [22, 23] for details). The geometry of the Bloch bundle for $d = 2$ is what enters in the theoretical understanding of the quantum Hall effect: the integer n that equals the Hall conductivity (1) in natural units is the (*first*) *Chern number* of $\mathscr{E}$, defined as

$$c_1(P) := \frac{1}{2\pi \mathrm{i}} \int_{\mathbb{T}^2} \operatorname{Tr}_{\mathscr{H}_\mathrm{f}} \left(P(k) \left[\partial_1 P(k), \partial_2 P(k)\right]\right) \mathrm{d}k_1 \mathrm{d}k_2 \quad \in \mathbb{Z}. \tag{2}$$

When $d = 2$, the above integer characterizes the isomorphism class of $\mathscr{E}$ as a vector bundle over $\mathbb{T}^2$ [23]. Since both quantum Hall and quantum spin Hall systems are 2-dimensional, in the following we will mostly restrict ourselves to $d = 2$, where in particular the previous characterization holds.

In the case where $\{P(k)\}_{k \in \mathbb{R}^d}$ satisfies also (P_3), then the Bloch bundle can be equipped with further structure, namely that of a fiberwise antilinear endomorphism $\widehat{\Theta}\colon \mathscr{E} \to \mathscr{E}$, lifting the involution $\theta(k) = -k$ on the base torus and squaring to the operator which multiplies fiberwise by -1. We call a vector bundle endowed with such an endomorphism $\widehat{\Theta}$ a *time-reversal symmetric vector bundle*. One can verify that if $d = 2$ every such vector bundle is trivial, i.e. isomorphic to the product bundle $\mathbb{T}^2 \times \mathbb{C}^m$, since under ($P_3$) the integrand in the definition (2) of the Chern number is an odd function of k, and hence integrates to zero on $\mathbb{T}^2$ [22, 23]. However, the Bloch bundle may still be non-trivial as time-reversal symmetric bundle [8, 10]. The index that characterizes the isomorphism class of $\mathscr{E}$ is the *Fu–Kane–Mele index* $\delta(P) \in \mathbb{Z}_2$, first introduced in [11] to describe quantum spin Hall systems. The expression of the $\mathbb{Z}_2$ index is slightly more involved than the one for the Chern number, and requires the introduction of some further terminology, which will be however essential in what follows.

Given a family of projectors $\{P(k)\}_{k \in \mathbb{R}^d}$ of constant rank m, a *Bloch frame* for it is a family of m-tuples of vectors $\Psi = \{\psi_a(k)\}_{1 \le a \le m,\, k \in \mathbb{R}^d}$, which are orthonormal and span the vector subspace $\operatorname{Ran} P(k) \subset \mathscr{H}_\mathrm{f}$ for all $k \in \mathbb{R}^d$. If $P(k)$ depends smoothly on k, then the same can be required of the frame Ψ. We immediately stress that, when $\{P(k)\}_{k \in \mathbb{R}^d}$ satisfies (P_1) and (P_2), then a Bloch frame is nothing but a trivializing frame for the associated Bloch bundle, and hence the existence of a continuous frame is in general guaranteed only *locally* in k. Let us also point out that, whenever a Bloch frame Ψ exists (say on an open domain $\Omega \subset \mathbb{R}^d$), then any

[2] In order for (P_2) and (P_3) to be compatible with each other, one should also require that $\tau_\lambda\, \Theta = \tau_\lambda^{-1}\, \Theta$ for all $\lambda \in \Lambda$. We will assume this in the following.

other Bloch frame Φ is obtained by setting

$$\phi_b(k) := \sum_{a=1}^{m} \psi_a(k)\, U(k)_{ab}, \quad 1 \le b \le m, \tag{3}$$

where $U(k)$, $k \in \Omega$, is a unitary matrix, called the *Bloch gauge*. We use the shorthand notation

$$\Phi(k) = \Psi(k) \triangleleft U(k), \quad k \in \Omega, \tag{4}$$

to write (3) in a more compact form. This defines a free right action of $\mathrm{U}(m)$ on frames, meaning that $(\Psi \triangleleft U_1) \triangleleft U_2 = \Psi \triangleleft (U_1\, U_2)$ and that $\Psi \triangleleft U_1 = \Psi \triangleleft U_2$ if and only if $U_1 = U_2$.

When a (local) Bloch frame $\Psi = \{\psi_a(k)\}_{1 \le a \le m,\, k \in \mathbb{R}^d}$ is given, then one can define the *Berry connection*, i.e. the matrix-valued 1-form given by

$$A = \left(\sum_{\mu=1}^{d} A_\mu(k)_{ab}\, \mathrm{d}k_\mu \right)_{1 \le a,b \le m}, \quad A_\mu(k)_{ab} := -\mathrm{i} \left\langle \psi_a(k), \partial_\mu \psi_b(k) \right\rangle. \tag{5}$$

This is indeed the matrix 1-form of the Grassmann connection on the Bloch bundle $\mathscr{E}$ (i.e. the pullback of the standard connection d via the obvious inclusion $\mathscr{E} \hookrightarrow \mathbb{T}^d \times \mathscr{H}_\mathrm{f}$), subordinated to the local trivialization induced by the choice of the Bloch frame. The *abelian* or $\mathrm{U}(1)$ *Berry connection* is then the trace of the connection matrix, namely

$$\mathscr{A} := \mathrm{Tr}(A) = \sum_{\mu=1}^{d} \mathscr{A}_\mu(k)\, \mathrm{d}k_\mu, \quad \mathscr{A}_\mu(k) := -\mathrm{i} \sum_{a=1}^{m} \left\langle \psi_a(k), \partial_\mu \psi_a(k) \right\rangle.$$

The *Berry curvature* 2-form is the curvature of the Berry connection, namely

$$F := \mathrm{d}A - \mathrm{i} \left[A \overset{\wedge}{,} A \right]$$

which spells out to

$$F = \sum_{1 \le \mu < \nu \le d} F_{\mu\nu}(k)\, \mathrm{d}k_\mu \wedge \mathrm{d}k_\nu,$$

$$F_{\mu\nu}(k) := \partial_\mu A_\nu(k) - \partial_\nu A_\mu - \mathrm{i} \left(A_\nu \wedge A_\mu - A_\mu \wedge A_\nu \right)$$

(the wedge product between matrix-valued 1-forms entails also the row-by-column product). Similarly, the *abelian* or U(1) *Berry curvature* is the trace

$$\mathscr{F} := \mathrm{Tr}(F) = \mathrm{d}\mathscr{A}. \tag{6}$$

In terms of the Bloch frame Ψ, the curvature $\mathscr{F}$ reads

$$\mathscr{F} = \sum_{1 \le \mu < \nu \le d} \mathscr{F}_{\mu\nu}(k)\, \mathrm{d}k_\mu \wedge \mathrm{d}k_\nu, \quad \mathscr{F}_{\mu\nu}(k) := 2\mathrm{Im}\left(\sum_{a=1}^{m} \left\langle \partial_\mu \psi_a(k), \partial_2 \psi_a(k) \right\rangle \right).$$

However, even if the Bloch frame is just a local object, the Berry curvature is a *global* one, as it can be expressed directly in terms of the family of projectors: a lengthy but straight-forward computation indeed shows that

$$\mathscr{F}_{\mu\nu}(k) = -\mathrm{i}\, \mathrm{Tr}_{\mathscr{H}_\mathrm{f}} \left(P(k) \left[\partial_\mu P(k), \partial_\nu P(k) \right] \right). \tag{7}$$

When $d = 2$, the above identity allows us to rewrite the Chern number as the integral of the (abelian) Berry curvature, namely

$$c_1(P) = \frac{1}{2\pi} \int_{\mathbb{T}^2} \mathscr{F} \quad \in \mathbb{Z} \tag{8}$$

[compare (2)]. Moreover, coming back to the Fu–Kane–Mele index of a time-reversal symmetric family of projectors, we can formulate $\delta(P) \in \mathbb{Z}_2$ through the notions we have just introduced as

$$\delta(P) := \frac{1}{2\pi} \int_{\mathbb{T}^2_+} \mathscr{F} - \frac{1}{2\pi} \int_{\partial \mathbb{T}^2_+} \mathscr{A} \mod 2 \tag{9}$$

where $\mathbb{T}^2_+$ denotes the set of points in $\mathbb{T}^2$ with non-negative k_1 coordinate [7, 11]. Remember that the Berry connection depends on the choice of a Bloch frame: for the above formula to be well-posed one must require that the Bloch frame be *time-reversal symmetric*, in a sense to be specified in the next Subsection. This point will be discussed further in Sect. 4.

Remark 1 (Gauge Dependence of Berry Connection and Curvature) For future reference, let us notice how the Berry connection and curvature matrices, as well as their abelian versions, change under a change of Bloch gauge. If Φ and Ψ are related by the gauge transformation U as in (4), their connection matrices A^Φ and

A^{Φ} are linked by the equation[3]

$$A^{\Phi} = U^{-1} A^{\Psi} U - \mathrm{i} U^{-1} \mathrm{d}U.$$

Taking the trace of both sides of the above equation we obtain the corresponding relation for the abelian Berry connections, namely

$$\mathscr{A}^{\Phi}(k) = \mathscr{A}^{\Psi}(k) - \mathrm{i}\,\mathrm{Tr}\left(U^{-1}\,\mathrm{d}U\right). \tag{10}$$

One can similarly compute that the Berry curvature is a gauge-covariant object, namely

$$F^{\Phi} = U^{-1} F^{\Psi} U,$$

and consequently the abelian Berry curvature $\mathscr{F}$ is gauge-invariant (namely $\mathscr{F}^{\Phi} = \mathscr{F}^{\Psi}$), as could be deduced already from its expression (7) given directly in terms of the projectors $P(k)$.

2.3 Obstruction Theory

Even though (2) and (9) express the Chern number and the Fu–Kane–Mele $\mathbb{Z}_2$ index by means of geometric objects related to the family of projectors (its Berry connection and Berry curvature, specifically), the fact that they indeed compute integers or integers mod 2 is a highly non-trivial statement. In the next Sections, we will deduce this fact by means of *obstruction theory*, a framework which allows

[3] An easy way to realize this is the following. The connection matrices $A^{\Psi}_{\mu}(k)$ and $A^{\Phi}_{\mu}(k)$ satisfy

$$\Psi(k) \triangleleft A^{\Psi}_{\mu}(k) = -\mathrm{i}\partial_{\mu}\Psi(k), \quad \Phi(k) \triangleleft A^{\Phi}_{\mu}(k) = -\mathrm{i}\partial_{\mu}\Phi(k).$$

As by definition we have $\Phi(k) = \Psi(k) \triangleleft U(k)$, we obtain

$$\begin{aligned} \Psi(k) \triangleleft (U(k)A^{\Phi}_{\mu}(k)) &= (\Psi(k) \triangleleft U(k)) \triangleleft A^{\Phi}_{\mu}(k) = \Phi(k) \triangleleft A^{\Phi}_{\mu}(k) = -\mathrm{i}\partial_{\mu}\Phi(k) \\ &= -\mathrm{i}\partial_{\mu}\left(\Psi(k) \triangleleft U(k)\right) = \left(-\mathrm{i}\partial_{\mu}\Psi(k)\right) \triangleleft U(k) + \Psi(k) \triangleleft \left(-\mathrm{i}\partial_{\mu}U(k)\right) \\ &= \left(\Psi(k) \triangleleft A^{\Psi}_{\mu}(k)\right) \triangleleft U(k) + \Psi(k) \triangleleft \left(-\mathrm{i}\partial_{\mu}U(k)\right) \\ &= \Psi(k) \triangleleft \left(A^{\Psi}_{\mu}(k)U(k) - \mathrm{i}\partial_{\mu}U(k)\right) \end{aligned}$$

by which we deduce that

$$U(k)A^{\Phi}_{\mu}(k) = A^{\Psi}_{\mu}(k)U(k) - \mathrm{i}\partial_{\mu}U(k).$$

to identify both indices as topological obstructions. This method has the advantage of manifesting both the quantization and the topological invariance of both indices, and requires only simple tools from linear algebra and basic topology.

Obstruction theory concerns the existence of a Bloch frame for a family of rank-m projectors $\{P(k)\}_{k\in\mathbb{R}^2}$ satisfying (P_1), (P_2) and, possibly, (P_3), which obeys the same symmetries of the projectors themselves. More specifically, we say that a Bloch frame Φ for $\{P(k)\}_{k\in\mathbb{R}^2}$ is

(F_1) *continuous* if the map $k \mapsto \Phi(k)$ is a continuous map from $\mathbb{R}^2$ to $\mathscr{H}_{\mathrm{f}}^m$;

(F_2) *τ-equivariant* if[4]

$$\Phi(k+\lambda) = \tau_\lambda\, \Phi(k) \quad \text{for all } k \in \mathbb{R}^2,\ \lambda \in \Lambda;$$

(F_3) *time-reversal symmetric* if[5]

$$\Phi(-k) = \Theta\Phi(k) \triangleleft \varepsilon$$

for a skew-symmetric unitary matrix ε. Without loss of generality [16], it can be assumed that

$$\varepsilon = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \oplus \overset{m/2 \text{ times}}{\cdots} \oplus \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{11}$$

The above properties in general compete against each other, as was early realized [11, 20] and as becomes apparent upon observing that a continuous, τ-equivariant (and time-reversal symmetric) Bloch frame would provide a global trivialization of the Bloch bundle as a (time-reversal symmetric) vector bundle.

The general strategy of obstruction theory consists in considering a continuous, globally defined Bloch frame Ψ, and trying to modify it in order to obtain a new Bloch frame Φ which satisfies also the properties of being τ-equivariant and, possibly, time-reversal symmetric. The input frame Ψ can be constructed by covering $\mathbb{R}^d$ with open balls $B_r(k_j)$, $r > 0$, $k_j \in \mathbb{R}^d$, in which $\left\| P(k) - P(k_j) \right\| < 1$, $k \in B_r(k_j)$, and using the Kato–Nagy unitary $U(k; k_j)$, which intertwines $P(k)$ and $P(k_j)$, to extend the choice of an orthonormal basis in the vector space $\operatorname{Ran} P(k_j)$ to a continuous choice of an orthonormal basis $\Psi(k)$ in $\operatorname{Ran} P(k)$ (that is, by definition, to a continuous Bloch frame on $B_r(k_j)$) [19]. An alternative construction makes use of the parallel transport associated to the family of projectors $P(k)$, see e.g. [7]. The modification of Ψ into Φ is performed by successive extensions, first at certain high-symmetry points, then along the edges that connect them, and finally on the whole

[4]The action of any (anti)unitary operator on $\mathscr{H}_{\mathrm{f}}$ is lifted to $\mathscr{H}_{\mathrm{f}}^m$ componentwise.

[5]The presence of the reshuffling matrix ε is needed to make the time-reversal symmetry condition self-consistent. This follows essentially from the fact that the antiunitary operator Θ defines by restriction a symplectic structure on the invariant subspace $\operatorname{Ran} P(k_\sharp) \subset \mathscr{H}_{\mathrm{f}}$ if $k_\sharp \equiv -k_\sharp \bmod \Lambda$. Notice that in particular the rank m of $P(k)$ must be even under (P_3).

$\mathbb{R}^2$. We will see that this latter step, from 1-dimensional lines to 2-dimensional faces, is in general topologically obstructed, and that this obstruction is encoded in the vanishing of the Chern number if one requires the Bloch frame Φ to satisfy (F_1) and (F_2) (see Sect. 3), or in the vanishing of the Fu–Kane–Mele index if one also requires (F_3) to hold (see Sect. 4).

Remark 2 (Analytic Bloch Frames) The obstruction to the existence of symmetric Bloch frames, being topological in nature, fits well inside the continuous category. However, one may wonder whether an analytic family of projectors as in (P_1) admits a Bloch frame depending *analytically* on k as well. This question is crucial in the study of conduction/insulation properties in crystals via *maximally localized Wannier functions* (see e.g. [4, 21]). There are by now several techniques that are able to construct analytic frames out of continuous ones preserving moreover all the symmetries, for example by convolution with suitable kernels [6, 7]. These are all incarnations of the more general *Oka's principle*, which states that in fair generality the obstruction to the triviality of a vector bundle in the continuous category can be lifted to the analytic one [23].

3 The Chern Number as a Topological Obstruction

In this section we illustrate how the Chern number in (2) encodes the topological obstruction to the existence of a continuous and τ-equivariant Bloch frame for a family of projectors $\{P(k)\}_{k\in\mathbb{R}^2}$ satisfying (P_1) and (P_2).

3.1 Reduction to the Unit Cell

The τ-covariance of the family of projectors allows one to focus on points k lying in the *fundamental unit cell* for the lattice $\Lambda = \mathrm{Span}_{\mathbb{Z}}\{e_1, e_2\}$, namely

$$\mathbb{B} := \left\{k = k_1e_1 + k_2e_2 \in \mathbb{R}^2 : |k_j| \le 1/2,\ 1 \le j \le 2\right\}.$$

Indeed, if one can find a continuous Bloch frame Φ on $\mathbb{B}$ such that $\Phi(k+\lambda) = \tau_\lambda\Phi(k)$ whenever $k \in \mathbb{B}$ and $\lambda \in \Lambda$ are such that $k + \lambda \in \mathbb{B}$ (a condition to be imposed on the boundary of the fundamental unit cell), then one can enforce τ-equivariance to extend the definition of Φ to the whole $\mathbb{R}^2$ in a continuous way. Conversely, the restriction Φ to $\mathbb{B}$ of a continuous, τ-equivariant Bloch frame defined on the whole $\mathbb{R}^2$ satisfies exactly the condition stated above.

As sketched in Sect. 2.3, the approach of obstruction theory starts from a Bloch frame Ψ defined on the unit cell. One then modifies its definition on the boundary of $\mathbb{B}$ in order to enforce τ-equivariance there, and then investigates whether it is possible to extend this modification continuously also on the interior of the unit cell. In particular, this construction on the boundary requires to take care of what happens at the four vertices of $\mathbb{B}$, namely the four points

$$v_1 = \left(-\frac{1}{2}, -\frac{1}{2}\right), \quad v_2 = \left(\frac{1}{2}, -\frac{1}{2}\right), \quad v_3 = \left(\frac{1}{2}, \frac{1}{2}\right), \quad v_4 = \left(-\frac{1}{2}, \frac{1}{2}\right).$$

If this procedure is successful, then the "output" frame $\Phi(k)$, $k \in \mathbb{B}$, will satisfy τ-equivariance on the boundary, and it will then be continuously extendable to the whole $\mathbb{R}^2$ by τ-equivariant continuation, as explained above.

Notice that both the input frame $\Psi(k)$ and the output frame $\Phi(k)$ give orthonormal bases for the vector space $\operatorname{Ran} P(k)$, hence they differ by the action of a unitary transformation (a Bloch gauge) $U(k) \in \mathrm{U}(m)$, as in (3). It is sometimes convenient to consider the continuous map $U \colon \mathbb{B} \to \mathrm{U}(m)$ as the unknown of the problem, rather than the Bloch frame Φ.

We will see that the only step of the construction of Φ which may be topologically obstructed is the "face" extension (from the boundary to the interior of $\mathbb{B}$), and that a quantitative measure of the presence of this topological obstruction is given by the Chern number of the family of projectors.

3.2 Bloch Frame on the Boundary

As a first step, we construct a continuous Bloch frame on the boundary of the fundamental unit cell which satisfies the τ-equivariance condition. The construction can be performed as follows. Given the reference frame $\Psi(v_1)$, one can consider its τ-translates $\tau_{e_1}\Psi(v_1)$ and $\tau_{e_2}\Psi(v_1)$, which constitute orthonormal bases in the subspaces $\operatorname{Ran} P(v_2)$ and $\operatorname{Ran} P(v_4)$, respectively. Let $U_{\mathrm{obs}}(v_2)$ (respectively $U_{\mathrm{obs}}(v_4)$) be the unitary matrix which maps the input frame $\Psi(v_2)$ (respectively $\Psi(v_4)$) to $\tau_{e_1}\Psi(v_1)$ (respectively $\tau_{e_2}\Psi(v_1)$):

$$\tau_{e_1}\Psi(v_1) = \Psi(v_2) \triangleleft U_{\mathrm{obs}}(v_2), \quad \tau_{e_2}\Psi(v_1) = \Psi(v_4) \triangleleft U_{\mathrm{obs}}(v_4).$$

If Ψ were already τ-equivariant then these *obstruction unitaries* would equal the identity matrix. Write $U_{\mathrm{obs}}(v_\sharp) = \mathrm{e}^{\mathrm{i}T(v_\sharp)}$, with $T(v_\sharp) = T(v_\sharp)^*$ self-adjoint, for $v_\sharp \in \{v_2, v_4\}$. Define moreover

$$\widehat{\Phi}(k) := \begin{cases} \Psi(k_1, -\frac{1}{2}) \triangleleft \mathrm{e}^{\mathrm{i}(2k_1+1)T(v_2)/2} & \text{if } k = (k_1, -\frac{1}{2}),\ k_1 \in [-\frac{1}{2}, \frac{1}{2}], \\ \tau_{e_1}\Psi(-\frac{1}{2}, k_2) \triangleleft \mathrm{e}^{\mathrm{i}(2k_2+1)T(v_4)/2} & \text{if } k = (\frac{1}{2}, k_2),\ k_2 \in [-\frac{1}{2}, \frac{1}{2}], \\ \tau_{e_2}\Psi(k_1, -\frac{1}{2}) \triangleleft \mathrm{e}^{\mathrm{i}(2k_1+1)T(v_2)/2} & \text{if } k = (k_1, \frac{1}{2}),\ k_1 \in [-\frac{1}{2}, \frac{1}{2}], \\ \Psi(-\frac{1}{2}, k_2) \triangleleft \mathrm{e}^{\mathrm{i}(2k_2+1)T(v_4)/2} & \text{if } k = (-\frac{1}{2}, k_2),\ k_2 \in [-\frac{1}{2}, \frac{1}{2}]. \end{cases} \tag{12}$$

The frame $\widehat{\Phi}$ is defined on the boundary $\partial\mathbb{B}$ of the fundamental unit cell, where it is also τ-equivariant. Moreover, it is continuous, as on the vertex v_3 the definitions coincide. Indeed we have

$$\tau_{e_1}\Psi(v_4) \triangleleft U_{\mathrm{obs}}(v_4) = \tau_{e_1}\tau_{e_2}\Psi(v_1) = \tau_{e_2}\tau_{e_1}\Psi(v_1) = \tau_{e_2}\Psi(v_2) \triangleleft U_{\mathrm{obs}}(v_2).$$

3.3 Extension to the Face: A Topological Obstruction

In order to see whether it is possible to extend the frame $\widehat{\Phi}$ to a continuous τ-equivariant Bloch frame Φ defined on the whole unit cell $\mathbb{B}$, we first introduce the unitary map $\widehat{U}(k)$ which maps the input frame $\Psi(k)$ to the frame $\widehat{\Phi}(k)$, i.e. such that

$$\widehat{\Phi}(k) = \Psi(k) \triangleleft \widehat{U}(k), \quad k \in \partial\mathbb{B} \tag{13}$$

[compare (3)]. This defines a continuous map $\widehat{U}\colon \partial\mathbb{B} \to \mathrm{U}(m)$. If we can find a continuous extension $U\colon \mathbb{B} \to \mathrm{U}(m)$ of $\widehat{U}$ to the unit cell, then (3) can be used to define an extension of the frame Φ which preserves continuity and τ-equivariance: it turns out that also the converse is true (compare Proposition 1 below).

It is a well-known fact in topology [9, Theorem 17.3.1] that a continuous map $\widehat{U}\colon \partial\mathbb{B} \to \mathrm{U}(m)$ extends continuously to the inside of the unit cell if and only if the map is homotopically trivial, i.e. it can be continuously deformed to a constant map. This condition can be checked by verifying that the integral

$$c := \deg([\widehat{U}]) = \frac{\mathrm{i}}{2\pi} \oint_{\partial\mathbb{B}} \mathrm{d}k \, \mathrm{Tr}\left(\widehat{U}(k)^{-1}\partial_k \widehat{U}(k)\right) \tag{14}$$

vanishes: this is because two maps $\partial\mathbb{B} \to \mathrm{U}(m)$ are homotopic if and only if their *degrees*, defined like in (14), coincide. Notice that the integral above gives an integer, and provides an isomorphism of the fundamental group $\pi_1(\mathrm{U}(m))$ (whose elements are homotopy classes of maps $\partial\mathbb{B} \to \mathrm{U}(m)$) with the group of integers $\mathbb{Z}$ by assigning $\widehat{U} \mapsto \deg([\widehat{U}])$ [17, Chap. 8, Sect. 12].

Remark 3 (Unwinding the Determinant is Forbidden) Since we have to extend the *frame* $\widehat{\Phi}$ rather than the *unitary* $\widehat{U}$, one may argue that it may be possible to find another unitary-matrix-valued map that "unwinds" the determinant of $\widehat{U}$, while preserving the relevant symmetries of the Bloch frame. This possibility is ruled out by the following result.

Proposition 1 *Let Φ be a continuous Bloch frame on $\partial\mathbb{B}$ which is τ-equivariant, and assume that $X\colon \partial\mathbb{B} \to \mathrm{U}(m)$ is a continuous map such that $\Phi \triangleleft X$ is also τ-equivariant. Then*

$$\deg([X]) = 0.$$

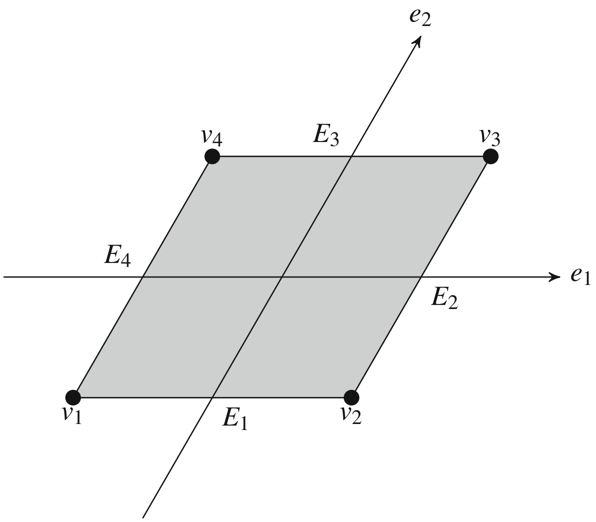

Fig. 1 The fundamental unit cell $\mathbb{B}$, its vertices and its edges

Proof We spell out what it means for Φ and $\Phi \triangleleft X$ to be both τ-equivariant:

$$\Phi(k+\lambda) \triangleleft X(k+\lambda) = \tau_\lambda\left(\Phi(k) \triangleleft X(k)\right) = \tau_\lambda \Phi(k) \triangleleft X(k) = \Phi(k+\lambda) \triangleleft X(k).$$

This implies that $X(k+\lambda) = X(k)$, whenever $k \in \partial\mathbb{B}$ and $\lambda \in \Lambda$ are such that $k+\lambda \in \partial\mathbb{B}$. As a consequence, the same is true for the expression $x(k) := \mathrm{Tr}\left(X(k)^{-1}\, \partial_k X(k)\right)$ appearing in the integral defining $\deg([X])$ [compare (14)]. Denote by E_i the edge of $\partial\mathbb{B}$ connecting v_i with $v_{(i+1) \bmod 4}$ (compare Fig. 1). Then the property $x(k+\lambda) = x(k)$ implies that

$$\int_{E_3} \mathrm{d}k\, x(k) = \int_{-(E_1+e_1)} \mathrm{d}k\, x(k) = -\int_{E_1} \mathrm{d}k\, x(k), \text{ that is } \int_{E_1+E_3} \mathrm{d}k\, x(k) = 0.$$

Similarly

$$\int_{E_2+E_4} \mathrm{d}k\, x(k) = 0.$$

We conclude that

$$\deg([X]) = \frac{\mathrm{i}}{2\pi} \int_{E_1+E_2+E_3+E_4} \mathrm{d}k\, x(k) = 0$$

as wanted.

3.4 The Obstruction is the Chern Number

We now want to rewrite the integer c in (14) and characterize it as a *topological invariant* of the family of projectors $\{P(k)\}_{k\in\mathbb{R}^2}$ [showing in particular that it does not depend on the input Bloch frame Ψ and on the specific interpolation performed on the obstruction matrices in (12)]. To this end, we will make use of the (abelian) Berry connection and curvature, introduced in Sect. 2.2.

If we calculate $\widehat{\mathscr{A}}$ on $\partial\mathbb{B}$ as in (5) using the vectors of the frame $\widehat{\Phi}$ and analogously compute $\mathscr{A}$ using Ψ, then

$$\widehat{\mathscr{A}} = \mathscr{A} - \mathrm{i}\,\mathrm{Tr}\left(\widehat{U}^{-1}\mathrm{d}\widehat{U}\right) \quad \text{on } \partial\mathbb{B}, \tag{15}$$

in view of (13) and (10). Integrating both sides of Eq. (15) on $\partial\mathbb{B}$, we obtain that

$$\begin{aligned} \frac{1}{2\pi}\oint_{\partial\mathbb{B}} \widehat{\mathscr{A}} &= \frac{1}{2\pi}\oint_{\partial\mathbb{B}} \mathscr{A} - \frac{\mathrm{i}}{2\pi}\oint_{\partial\mathbb{B}} \mathrm{d}k\; \mathrm{Tr}\left(\widehat{U}(k)^{-1}\partial_k\widehat{U}(k)\right) \\ &= \left(\frac{1}{2\pi}\int_{\mathbb{B}}\mathscr{F}\right) - c \end{aligned} \tag{16}$$

by (6) and Stokes theorem.

We will now show that the left-hand side of the above equality vanishes. In order to do so, we exploit the τ-equivariance of the Bloch frame $\widehat{\Phi}$, that is, $\widehat{\Phi}(k+\lambda) = \tau_\lambda\widehat{\Phi}(k)$. Indeed, in terms of the Berry connection matrix $A = A(k)\,\mathrm{d}k$ we have that

$$\begin{aligned} \widehat{\Phi}(k+\lambda) \triangleleft \widehat{A}(k+\lambda) &= -\mathrm{i}\partial_k\widehat{\Phi}(k+\lambda) = \tau_\lambda\left(-\mathrm{i}\partial_k\widehat{\Phi}(k)\right) \\ &= \tau_\lambda\left(\widehat{\Phi}(k+\lambda) \triangleleft \widehat{A}(k)\right) = \tau_\lambda\widehat{\Phi}(k+\lambda) \triangleleft \widehat{A}(k) \\ &= \widehat{\Phi}(k+\lambda) \triangleleft \widehat{A}(k) \end{aligned} \tag{17}$$

so that $\widehat{A}(k+\lambda) = \widehat{A}(k)$ and, taking the trace, $\widehat{\mathscr{A}}(k+\lambda) = \widehat{\mathscr{A}}(k)$. Arguing similarly to the proof of Proposition 1, one can show that the latter relation implies

$$\int_{E_1+E_3} \widehat{\mathscr{A}} = 0, \quad \int_{E_2+E_4} \widehat{\mathscr{A}} = 0,$$

yielding the vanishing of the left-hand side of (16).

Hence we conclude that

$$\left(\frac{1}{2\pi}\int_{\mathbb{B}}\mathscr{F}\right) - c = \frac{1}{2\pi}\oint_{\partial\mathbb{B}} \widehat{\mathscr{A}} = 0$$

which in view of (8) yields

$$c = \frac{1}{2\pi} \int_{\mathbb{B}} \mathscr{F} = c_1(P) \tag{18}$$

as wanted.

4 The Fu–Kane–Mele Invariant as a Topological Obstruction

In this Section, we switch to the time-reversal symmetric setting. As was already mentioned, in this case the presence of a further symmetry kills the topological obstruction given by the Chern number (2) [22, 23]. However, the same symmetry allows to refine the notion of "symmetric Bloch frame" by requiring that it be also time-reversal symmetric (compare Sect. 2.3). This gives rise to a new topological obstruction encoded in the Fu–Kane–Mele $\mathbb{Z}_2$ invariant [10, 11], as we will now show.

Throughout this section, $\{P(k)\}_{k\in\mathbb{R}^2}$ denotes a family of orthogonal projectors satisfying (P_1), (P_2) and (P_3).

4.1 Reduction to the Effective Unit Cell

In order to investigate the existence of a global Bloch frame for $P(k)$ which is continuous, τ-equivariant, and time-reversal symmetric, it is sufficient to focus one's attention to momenta in the *effective unit cell* for the lattice $\Lambda = \mathrm{Span}_{\mathbb{Z}}\{e_1, e_2\}$, defined as

$$\mathbb{B}_{\mathrm{eff}} := \left\{k = k_1 e_1 + k_2 e_2 \in \mathbb{R}^2 : 0 \le k_1 \le 1/2,\ -1/2 \le k_2 \le 1/2\right\}.$$

Indeed, all points of $\mathbb{R}^2$ can be mapped to $\mathbb{B}_{\mathrm{eff}}$ (in an a.e. unique way) by means of a combination of a translation $k \mapsto k + \lambda$, $\lambda \in \Lambda$, and possibly an inversion $k \mapsto -k$. This means that if a Bloch frame is defined on $\mathbb{B}_{\mathrm{eff}}$ and satisfies the relevant symmetries there, then it is possible to extend its definition first to the unit cell $\mathbb{B}$ by enforcing time-reversal symmetry, and secondly to the whole $\mathbb{R}^2$ imposing τ-equivariance. This dictates that the required frame Φ on $\mathbb{B}_{\mathrm{eff}}$ satisfies certain compatibility conditions on the boundary of the effective unit cell, namely that $\Phi(k+\lambda) = \tau_\lambda \Phi(k)$ and $\Phi(-k) = \Theta\Phi(k) \triangleleft \varepsilon$, whenever $k \in \partial\mathbb{B}_{\mathrm{eff}}$ and $\lambda \in \Lambda$ are such that $\pm k + \lambda \in \partial\mathbb{B}_{\mathrm{eff}}$.

We will again resort to the technique of obstruction theory. Consequently, we will choose a continuous Bloch frame Ψ on $\mathbb{B}_{\mathrm{eff}}$, and try to modify it into a frame Φ satisfying the symmetries mentioned above. The two frames $\Psi(k)$ and $\Phi(k)$ will be related by a unitary transformation, which we denote by $U(k)$ as in (3). As in

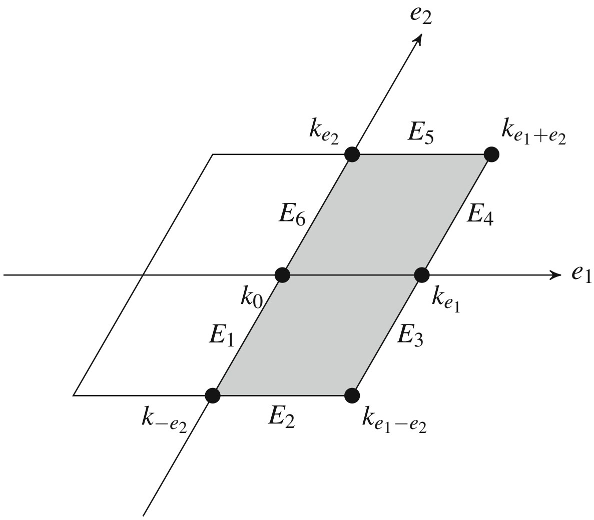

Fig. 2 The effective unit cell $\mathbb{B}_{\text{eff}}$ and the time-reversal invariant momenta

Sect. 3.1, a special role is played by the high-symmetry points k_λ, defined by the relation $k_\lambda + \lambda = -k_\lambda$ with $\lambda \in \Lambda$ (that is, $k_\lambda = \lambda/2$). Six such points lie on the boundary of $\mathbb{B}_{\text{eff}}$, and are usually referred to as the *time-reversal invariant momenta* (compare Fig. 2).

4.2 Bloch Frame on the Boundary

As a first step, we provide here the construction of a symmetric Bloch frame defined on the boundary of the effective unit cell $\mathbb{B}_{\text{eff}}$, following the obstruction-theoretic approach employed in the previous Section for the non-time-reversal-symmetric case.

Let k_λ be any of the time-reversal invariant momenta. Given the input frame $\Psi(k_\lambda)$, the transformed frames $\Theta\Psi(k_\lambda) \triangleleft \varepsilon$ and $\tau_\lambda \Psi(k_\lambda)\Psi(k_\lambda)$ both give bases of the same vector space $\operatorname{Ran} P(-k_\lambda) = \operatorname{Ran} P(k_\lambda + \lambda)$. As such, they must differ by the action of an *obstruction unitary* matrix:

$$\Theta\Psi(k_\lambda) \triangleleft \varepsilon = \tau_\lambda \Psi(k_\lambda) \triangleleft U_{\text{obs}}(k_\lambda). \tag{19}$$

These unitary matrices satisfy a further self-compatibility condition, namely

$$U_{\text{obs}}(k_\lambda)^{\mathsf{T}}\, \varepsilon = \varepsilon\, U_{\text{obs}}(k_\lambda), \tag{20}$$

as can be deduced from the following considerations. Applying the operator $\tau_\lambda \Theta = \Theta \tau_\lambda^{-1}$ to both sides of the identity (19), and using the defining properties of the time-reversal operator Θ, we obtain

$$\tau_\lambda \Psi(k_\lambda) \triangleleft (-\overline{\varepsilon}) = \Theta \Psi(k_\lambda) \triangleleft \overline{U_{\rm obs}(k_\lambda)}.$$

Using the relation (19) again we can rewrite the above equality as

$$\Theta \Psi(k_\lambda) \triangleleft \left(-\varepsilon\, U_{\rm obs}(k_\lambda)^{-1}\, \overline{\varepsilon}\right) = \Theta \Psi(k_\lambda) \triangleleft \overline{U_{\rm obs}(k_\lambda)}$$

from which we deduce that $-\varepsilon\, U_{\rm obs}(k_\lambda)^{-1}\, \overline{\varepsilon} = \overline{U_{\rm obs}(k_\lambda)}$. Taking complex conjugates and using the fact that $-\overline{\varepsilon} = \varepsilon^{-1}$ (by unitarity and skew-symmetry) yields exactly (20).

Write now $U_{\rm obs}(v_\sharp) = \mathrm{e}^{\mathrm{i}T(v_\sharp)}$ for $v_\sharp \in \{v_1, \dots, v_4\}$, with $T(v_\sharp) = T(v_\sharp)^*$ self-adjoint and satisfying $\sigma(T(v_\sharp)) \subset (-\pi, \pi]$. This normalization on the arguments of the eigenvalues of $U_{\rm obs}(v_\sharp)$ gives that $T(v_\sharp)$ inherits the property (20) in the form

$$T(v_\sharp)^{\mathsf{T}}\, \varepsilon = \varepsilon\, T(v_\sharp) \tag{21}$$

(see [16, Sect. 6, Lemma]).

Set now

$$\widehat{\Phi}(k) := \begin{cases} \Psi(k) \triangleleft V(k) & \text{if } k \in S, \\ \tau_{e_1}^{-1} \Theta \Psi(\frac{1}{2}, -k_2) \triangleleft \left(\overline{V(\frac{1}{2}, -k_2)}\, \varepsilon\right) & \text{if } k = (\frac{1}{2}, k_2),\ k_2 \in [0, \frac{1}{2}], \\ \tau_{e_2} \Psi(k_1, -\frac{1}{2}) \triangleleft V(k_1, -\frac{1}{2}) & \text{if } k = (k_1, \frac{1}{2}),\ k_1 \in [0, \frac{1}{2}], \\ \Theta \Psi(0, -k_2) \triangleleft \left(\overline{V(0, -k_2)}\, \varepsilon\right) & \text{if } k = (0, k_2),\ k_2 \in [0, \frac{1}{2}], \end{cases} \tag{22}$$

where

$$S := \left\{k = (0, k_2) : k_2 \in \left[-\tfrac{1}{2}, 0\right]\right\} \cup \left\{k = \left(k_1, -\tfrac{1}{2}\right) : k_1 \in \left[0, \tfrac{1}{2}\right]\right\} \\ \cup \left\{k = \left(\tfrac{1}{2}, k_2\right) : k_2 \in \left[-\tfrac{1}{2}, 0\right]\right\}$$

and for $k \in S$

$$V(k) := \begin{cases} \mathrm{e}^{\mathrm{i}[(1+2k_2)T(v_1) - 2k_2 T(v_2)]/2} & \text{if } k = (0, k_2),\ k_2 \in [-\frac{1}{2}, 0], \\ \mathrm{e}^{\mathrm{i}[(1-2k_1)T(v_2) + 2k_1 T(v_3)]/2} & \text{if } k = (k_1, -\frac{1}{2}),\ k_1 \in [-\frac{1}{2}, 0], \\ \mathrm{e}^{\mathrm{i}[(1+2k_2)T(v_3) - 2k_2 T(v_4)]/2} & \text{if } k = (\frac{1}{2}, k_2),\ k_2 \in [-\frac{1}{2}, 0]. \end{cases} \tag{23}$$

Equation (22) above defines a Bloch frame $\widehat{\Phi}$ on $\partial \mathbb{B}_{\rm eff}$ which is by construction τ-equivariant and time-reversal symmetric. Notice also that (23) yields

$$U_{\rm obs}(k_\lambda) = V(k_\lambda)^2 = V(k_\lambda) \varepsilon^{-1} V(k_\lambda)^{\mathsf{T}} \varepsilon$$

at the time-reversal invariant momenta. Repeated use of the defining property (19) for $U_{\mathrm{obs}}(k_\lambda)$ and of its generator $T(k_\lambda)$, together with (20) and (21), shows that $\widehat{\Phi}$ also joins continuously at the time-reversal invariant momenta. For example, at $k_\lambda = k_{e_1} = (1/2, 0)$ we have

$$\begin{aligned}\tau_{e_1}^{-1} \Theta\Psi(k_{e_1}) \triangleleft \left(\overline{V(k_{e_1})}\,\varepsilon\right) &= \tau_{e_1}^{-1} \Theta\Psi(k_{e_1}) \triangleleft \left(\varepsilon\, V(k_{e_1})^*\right) \\ &= \tau_{e_1}^{-1} \left(\Theta\Psi(k_{e_1}) \triangleleft \varepsilon\right) \triangleleft V(k_{e_1})^* \\ &= \tau_{e_1}^{-1} \left(\tau_{e_1}\Psi(k_{e_1}) \triangleleft U_{\mathrm{obs}}(k_{e_1})\right) \triangleleft V(k_{e_1})^{-1} \\ &= \Psi(k_{e_1}) \triangleleft \left(V(k_{e_1})^2 V(k_{e_1})^{-1}\right) = \Psi(k_{e_1}) \triangleleft V(k_{e_1}).\end{aligned}$$

4.3 Extension to the Face: A Topological Obstruction

Let $\widehat{U}$ denote the unitary transformation mapping the input frame Ψ to the Bloch frame $\widehat{\Phi}$ we just constructed, as in (13). We have already argued in the previous Section that the obstruction to the continuous extension of the map $\widehat{U}\colon \partial\mathbb{B}_{\mathrm{eff}} \to \mathrm{U}(m)$ to the interior of the effective unit cell is measured precisely by the vanishing of the integer $\deg([\widehat{U}]) \in \mathbb{Z}$ given by

$$\deg([\widehat{U}]) = \frac{\mathrm{i}}{2\pi} \oint_{\partial\mathbb{B}_{\mathrm{eff}}} \mathrm{d}k\, \mathrm{Tr}\left(\widehat{U}(k)^{-1} \partial_k \widehat{U}(k)\right) \tag{24}$$

[compare (14)]. However, in this new setting it is no longer the case that the extension problem for the unitary $\widehat{U}$ is equivalent to the one for the frame $\widehat{\Phi}$, as opposed to the situation in Remark 3. Indeed, we have the following result.

Proposition 2 *Let Φ be a continuous Bloch frame on $\partial\mathbb{B}_{\mathit{eff}}$ which is symmetric, and assume that $X\colon \partial\mathbb{B}_{\mathit{eff}} \to \mathrm{U}(m)$ is a continuous map such that $\Phi \triangleleft X$ is also symmetric. Then*

$$\deg([X]) \in 2\mathbb{Z}.$$

Proof One easily computes that asking that $\Phi \triangleleft X$ be again τ-equivariant and time-reversal symmetric is equivalent to the conditions

$$X(k+\lambda) = X(k) \quad \text{and} \quad X(-k+\lambda)^{\mathsf{T}}\, \varepsilon\, X(k) = \varepsilon \tag{25}$$

whenever $k \in \partial\mathbb{B}_{\mathrm{eff}}$ and $\lambda \in \Lambda$ are such that $\pm k + \lambda \in \partial\mathbb{B}_{\mathrm{eff}}$. In view of the above conditions, the integral computing the degree of X, as in (24), simplifies to

$$\deg([X]) = 2\left\{\frac{\mathrm{i}}{2\pi}\int_{E_1} \mathrm{d}k\, \mathrm{Tr}\left(X(k)^{-1}\partial_k X(k)\right) + \frac{\mathrm{i}}{2\pi}\int_{E_3} \mathrm{d}k\, \mathrm{Tr}\left(X(k)^{-1}\partial_k X(k)\right)\right\} \tag{26}$$

where the E_i's are the portions of $\partial\mathbb{B}_{\text{eff}}$ connecting two consecutive time-reversal invariant momenta (compare Fig. 2).

Notice now that for a unitary-matrix-valued map

$$\operatorname{Tr}\left(X(k)^{-1}\partial_k X(k)\right) = \xi(k)^{-1}\partial_k \xi(k), \quad \text{with } \xi(k) = \det X(k) \in U(1)$$

(see e.g. [7, Lemma 2.12]). On E_1 and E_3, the maps $k \mapsto \xi(k)$ are actually periodic, since the second condition in (25) implies that at the time-reversal invariant momenta k_λ the matrix $X(k_\lambda)$ must be symplectic and thus of unit determinant. The term in curly brackets on the right-hand side of (26) then computes the sum of the winding numbers of the maps $\xi\big|_{E_1}$ and $\xi\big|_{E_3}$, and is thus an integer. This concludes the proof of the Proposition.

The above result shows that if $\deg([\widehat{U}]) = 2r \in 2\mathbb{Z}$ is even, it is still possible to "unwind" the map $\widehat{U}$ with the help of an auxiliary map X, without breaking the symmetries (τ-equivariance, time-reversal) enjoyed by the frame $\widehat{\Phi}$ as in (22). Indeed, it is easily verified that the map $X\colon \partial\mathbb{B}_{\text{eff}} \to \mathrm{U}(m)$ defined (in the basis where ε is of the form (11)) by

$$X(k) = \begin{cases} \mathrm{e}^{-2\pi\mathrm{i}r(k_2+1/2)}\mathbb{1}_2 \oplus \mathbb{1}_{m-2} & \text{if } k = (\frac{1}{2}, k_2) \in E_3 \cup E_4,\ k_2 \in [-\frac{1}{2}, \frac{1}{2}], \\ \mathbb{1}_m & \text{elsewhere in } \partial\mathbb{B}_{\text{eff}}, \end{cases}$$

satisfies (25) and $\deg([X]) = -2r$. It follows that the frame $\Psi \triangleleft (\widehat{U}X)$ is still continuous, τ-equivariant and time-reversal symmetric, and extends to a continuous Bloch frame Φ in the interior of $\mathbb{B}_{\text{eff}}$ since $\deg([\widehat{U}X]) = 0$.

We conclude that the topological obstruction to the existence of a continuous and symmetric Bloch frame is measured by the quantity

$$d := \deg([\widehat{U}]) \mod 2. \tag{27}$$

It can be shown [10] that $d \in \mathbb{Z}_2$ defines a true *topological invariant* for the family of projectors $P(k)$ enjoying (P_1), (P_2) and (P_3), that is, it does not depend on the choice of the input frame Ψ and on the explicit form of the interpolation V as in (23), and moreover it stays constant under continuous deformations (homotopies) of the family of projectors which preserve its symmetry properties.

4.4 The Obstruction is the Fu–Kane–Mele Index

Arguing along the same lines of Sect. 3.4, it is possible to write the topological invariant d in terms of the Berry connection and the Berry curvature associated to the family of projectors $P(k)$, which in turn connects d with the Fu–Kane–Mele $\mathbb{Z}_2$ index for time-reversal symmetric topological insulators [11]. Indeed, the analogue of (16) reads now

$$\delta = \frac{1}{2\pi}\int_{\mathbb{B}_{\text{eff}}} \mathscr{F} - \frac{1}{2\pi}\oint_{\partial\mathbb{B}_{\text{eff}}} \widehat{\mathscr{A}} \mod 2 = \delta(P), \tag{28}$$

compare (9). Let us stress that the Berry connection $\widehat{\mathscr{A}}$ appearing in the above formula must be computed with respect to a frame $\widehat{\Phi}$ which is τ-equivariant *and time-reversal symmetric* on the boundary of the effective unit cell $\mathbb{B}_{\text{eff}}$. This guarantees, for example, that the expression on the right-hand side is gauge-independent, as we have seen how a change of unitary gauge which preserves the symmetries must have even degree (Proposition 2).

Notice that, contrary to the case of the Chern number treated in Sect. 3.4, the "boundary term" in (28) need not vanish. Indeed, the symmetries

$$\widehat{\mathscr{A}}(k+\lambda) = \widehat{\mathscr{A}}(k) = \widehat{\mathscr{A}}(-k) \tag{29}$$

of the coefficient of the Berry connection 1-form, which are inherited from the τ-equivariance and the time-reversal symmetry of the underlying frame $\widehat{\Phi}$, only imply that its integral on $\partial\mathbb{B}_{\text{eff}}$ can be simplified to

$$\oint_{\partial\mathbb{B}_{\text{eff}}} \widehat{\mathscr{A}} = 2\int_{E_1+E_3} \widehat{\mathscr{A}} = 2\left(\int_0^{1/2} \mathrm{d}k_2 \left[\widehat{\mathscr{A}}(1/2,k_2) - \widehat{\mathscr{A}}(0,k_2)\right]\right).$$

The first equality in (29) can be argued exactly as in (17), while for the second one we proceed as follows. From the time-reversal symmetry property $\widehat{\Phi}(-k) = \Theta\widehat{\Phi}(k) \triangleleft \varepsilon$ it follows that

$$\Theta\left(\partial_k\widehat{\Phi}(k)\right) \triangleleft \varepsilon = -\left(\partial_k\widehat{\Phi}\right)(-k).$$

Using the relation above together with the defining property $\widehat{\Phi}(k) \triangleleft \widehat{A}(k) = -\mathrm{i}\partial_k\widehat{\Phi}(k)$ for the connection matrix $\widehat{A}(k)$ we then obtain

$$\begin{aligned}\Theta\widehat{\Phi}(k) \triangleleft \left(\varepsilon\widehat{A}(-k)\right) &= \widehat{\Phi}(-k) \triangleleft \widehat{A}(-k) = -\mathrm{i}\left(\partial_k\widehat{\Phi}\right)(-k) \\ &= \mathrm{i}\Theta\left(\partial_k\widehat{\Phi}(k)\right) \triangleleft \varepsilon = \Theta\left(-\mathrm{i}\partial_k\widehat{\Phi}(k)\right) \triangleleft \varepsilon \\ &= \Theta\left(\widehat{\Phi}(k) \triangleleft \widehat{A}(k)\right) \triangleleft \varepsilon = \Theta\widehat{\Phi}(k) \triangleleft \left(\overline{\widehat{A}(k)}\varepsilon\right).\end{aligned}$$

We conclude that $\widehat{A}(-k) = \varepsilon^{-1}\overline{\widehat{A}(k)}\varepsilon$, and by taking the trace that $\widehat{\mathscr{A}}(-k) = \overline{\widehat{\mathscr{A}}(k)} = \widehat{\mathscr{A}}(k)$, because $\widehat{\mathscr{A}}(k)$ takes values in the Lie algebra $\mathfrak{u}(1) = \mathbb{R}$.

Acknowledgements The author is indebted with D. Fiorenza and G. Panati for valuable discussions, as well as with G. dell'Antonio and A. Michelangeli for the invitation to the INdAM meeting "Contemporary Trends in the Mathematics of Quantum Mechanics". Financial support from INdAM and from the German Science Foundation (DFG) within the GRK 1838 "Spectral theory and dynamics of quantum systems" is gratefully acknowledged.

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Norm Approximation for Many-Body Quantum Dynamics and Bogoliubov Theory

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Abstract We review some recent results on the norm approximation to the Schrödinger dynamics. We consider N bosons in $\mathbb{R}^3$ with an interaction potential of the form $N^{3\beta-1}w(N^\beta(x-y))$ with $0 \leq \beta < 1/2$, and show that in the large N limit, the fluctuations around the condensate can be effectively described using Bogoliubov approximation.

Keywords Bogoliubov approximation • Bose-Einstein condensation • Many body quantum dynamics

1 Introduction

In 1924–1925, Bose [10] and Einstein [14] predicted that at a very low temperature, many bosons condense into a common quantum state. It took 70 years until this phenomenon was first observed by Cornell, Wieman and Ketterle [3, 12]. Since then, many interesting questions remain unsolved from the theoretical point of view. In fact, Bose and Einstein only considered the ideal gas. The study of interacting Bose gas was initiated in 1947 by Bogoliubov [9]. Roughly speaking, Bogoliubov theory is based on the reduction to quasi-free particles, which can be seen as the bosonic analogue to the Bardeen–Cooper–Schrieffer theory [5] for superconductivity.

In the last decades, there have been many attempts to justify Bogoliubov theory from the first principles of quantum mechanics, namely from Schrödinger equation. In the context of the ground state problem, this has been done successfully for one and two-component Bose gases [33, 34, 47], for the Lee-Huang-Yang formula of homogeneous, dilute gases [19, 27, 49] and for the excitation spectrum in the

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A. Michelangeli, G. Dell'Antonio (eds.), *Advances in Quantum Mechanics*,
Springer INdAM Series 18, DOI 10.1007/978-3-319-58904-6_13

mean-field regime [13, 22, 31, 41, 46]. In the context of the dynamical problem, Bogoliubov theory has been used widely to study the quantum dynamics of coherent states in Fock space [8, 20, 21, 23–26, 28, 29, 45]. Very recently, Lewin, Schlein and one of us [30] were able to justify Bogoliubov theory as a norm approximation for the N-particle quantum dynamics in the mean-field regime. In [39, 40], we revisited the approach in [30] and extended it to the case of a dilute gas. In the following, we will review our results in [39, 40] and explain the ideas of the proof.

We consider a system of N bosons in $\mathbb{R}^3$, described by a wave function $\Psi_N(t)$ in the Hilbert space $\mathfrak{H}^N = \bigotimes_{\text{sym}}^N L^2(\mathbb{R}^3)$. The system is governed by Schrödinger equation $\Psi_N(t) = e^{-itH_N}\Psi_N(0)$ with a typical N-body Hamiltonian

$$H_N = \sum_{j=1}^N -\Delta_{x_j} + \frac{1}{N-1} \sum_{1\le j<k\le N} w_N(x_j - x_k).$$

We are interested in the delta-type interaction

$$w_N(x-y) = N^{3\beta} w(N^\beta(x-y))$$

where $w \ge 0$ is a fixed function which is smooth, radially symmetric, decreasing and with compact support. We put the coupling constant $1/(N-1)$ in order to make the kinetic energy and interaction energy comparable in the large N limit.

The parameter $\beta \ge 0$ describes the character of the interaction between the particles. In the mean-field regime $\beta < 1/3$, there are many but weak collisions and it is naturally to treat the particles as if they were independent but subjected to a common self-consistent mean-field potential. In the dilute regime $\beta > 1/3$, there are few but strong collisions and the particles are more correlated. The latter regime is more relevant physically, but also more difficult mathematically.

Our motivation is that $\Psi_N(0)$ is the ground state of a trapped system and the time evolution $\Psi_N(t)$ is observed when the trapping potential is turned off. From the rigorous result on the ground state in [31], we will assume that

$$\Psi_N(0) = \sum_{n=0}^N u(0)^{\otimes(N-n)} \otimes_s \varphi_n(0) = \sum_{n=0}^N \frac{(a^*(u(0)))^{N-n}}{\sqrt{(N-n)!}} \varphi_n(0) \tag{1}$$

where $u(0)$ is a normalized function in $L^2(\mathbb{R}^3)$ which describes the condensate and $\Phi(0) = (\varphi_n(0))_{n=0}^\infty$ is a state in the Fock space of the excited particles. Here we use the usual notations of the annihilation and creation operators

$$a^*(f) = \int_{\mathbb{R}^3} f(x) a_x^* \,\mathrm{d}x, \quad a(f) = \int_{\mathbb{R}^3} \overline{f(x)} a_x \,\mathrm{d}x, \quad \forall f \in \mathfrak{H},$$

where the operator valued distributions a_x and a_x^* satisfy $[a_x^*, a_y^*] = [a_x, a_y] = 0$, $[a_x, a_y^*] = \delta(x-y)$.

When $\beta = 0$, it was shown in [30] that if (1) holds then

$$\lim_{N\to\infty} \left\| \Psi_N(t) - \sum_{n=0}^{N} u(t)^{\otimes(N-n)} \otimes_s \varphi_n(t) \right\| = 0 \tag{2}$$

(see also the recent work [38] for another approach). Here $u(t)$ is the evolution of the condensate, governed by the (N-dependent) Hartree equation

$$i\partial_t u(t) = \big(-\Delta + w_N * |u(t)|^2 - \mu_N(t)\big)u(t), \quad u(t=0) = u(0). \tag{3}$$

The phase parameter $\mu_N(t)$ plays the role of the chemical potential and it can be chosen as

$$\mu_N(t) = \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} |u(t,x)|^2 w_N(x-y)|u(t,y)|^2 \,\mathrm{d}x\,\mathrm{d}y.$$

The vector $\Phi(t) = (\varphi_n(t))_{n=0}^{\infty}$ in (2) is a state in the excited Fock space

$$\mathscr{F}_+(t) = \bigoplus_{n=0}^{\infty} \mathfrak{H}_+(t)^n, \quad \mathfrak{H}_+(t)^n = \bigotimes_{\text{sym}}^{n} \{u(t)\}^\perp$$

and it is determined by Bogoliubov equation

$$i\partial_t \Phi(t) = \mathbb{H}(t)\Phi(t), \quad \Phi(t=0) = \Phi(0). \tag{4}$$

Here $\mathbb{H}(t)$ is a quadratic Hamiltonian in Fock space:

$$\mathbb{H}(t) = \mathrm{d}\Gamma(h(t)) + \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \Big(K_2(t,x,y)a_x^* a_y^* + \overline{K_2(t,x,y)}a_x a_y\Big)\,\mathrm{d}x\ \mathrm{d}y,$$

which is obtained from Bogoliubov approximation (which we will explain in Sect. 2). We use the notations $\mathrm{d}\Gamma(A) = \int a_x^* A_x a_x \,\mathrm{d}x$ (for example, $\mathrm{d}\Gamma(1) = \mathscr{N}$ is the number operator) and

$$h(t) = -\Delta + |u(t,\cdot)|^2 * w_N - \mu_N(t) + Q(t)\widetilde{K}_1(t)Q(t),$$
$$K_2(t) = Q(t) \otimes Q(t)\widetilde{K}_2(t), \quad Q(t) = 1 - |u(t)\rangle\langle u(t)|,$$

where $\widetilde{K}_2(t,x,y) = u(t,x)w_N(x-y)u(t,y)$ is a function in $\mathfrak{H}^2$ and $\widetilde{K}_1(t)$ is an operator on $\mathfrak{H}$ with kernel $\widetilde{K}_1(t,x,y) = u(t,x)w_N(x-y)\overline{u(t,y)}$.

In order to extend (2) to the case $\beta > 0$, we have to restrict the initial state $\Phi(0)$ in (1) to quasi-free states (namely the states satisfying Wick theorem) with finite kinetic energy. This reduction is again admissible by the rigorous properties of ground states in [31] (in fact, $\Phi(0)$ is the ground state of a quadratic Hamiltonian on Fock space, and hence it is a quasi-free state with finite kinetic energy). Our main result in [40] is

Theorem 1 (Validity of Bogoliubov Theory as a Norm Approximation) *Let $\Psi_N(t) = e^{-itH_N}\Psi_N(0)$ with $\Psi_N(0)$ given in (1). We assume*

- *$u(t)$ satisfies Hartree equation (3) with the (possibly N-dependent) initial state $u(0,\cdot)$ satisfying $\|u(0,\cdot)\|_{W^{\ell,1}(\mathbb{R}^3)} \le C$ for ℓ sufficiently large;*
- *$\Phi(t) = (\varphi_n(t))_{n=0}^\infty \in \mathscr{F}_+(t)$ satisfies Bogoliubov equation (4) (or equivalently, Eq. (12) in Sect. 2) with the (possibly N-dependent) initial state $\Phi(0)$ being a quasi-free state in $\mathscr{F}_+(0)$ such that for all $\varepsilon > 0$,*

$$\left\langle \Phi(0), \mathscr{N}\Phi(0)\right\rangle \le C_\varepsilon N^\varepsilon, \quad \left\langle \Phi(0), \mathrm{d}\Gamma(1-\Delta)\Phi(0)\right\rangle \le C_\varepsilon N^{\beta+\varepsilon}. \tag{5}$$

Then for all $0 \le \beta < 1/2$, all $\varepsilon > 0$ and all $t > 0$ we have

$$\left\| \Psi_N(t) - \sum_{n=0}^{N} u(t)^{\otimes(N-n)} \otimes_s \varphi_n(t) \right\|_{\mathfrak{H}^N}^2 \le C_\varepsilon (1+t)^{1+\varepsilon} N^{(2\beta-1+\varepsilon)/2}. \tag{6}$$

Convention We always denote by C (or C_ε) a general positive constant independent of N and t (C_ε may depend on ε).

There are grand canonical analogues of (2) related to the fluctuations around coherent states in Fock space [20, 21, 23, 25, 26, 28, 29]. In particular, our Theorem 1 is comparable to the Fock-space result of Kuz [29]. Thanks to a heuristic argument in [29], the range $0 \le \beta < 1/2$ is optimal for the norm approximation (2) to hold.

When $\beta > 1/2$, to achieve (2) we have to modify the effective equations to take two-body scattering processes into account. This has been done in the Fock space setting by Boccato, Cenatiempo and Schlein [8] and Grillakis and Machedon [24] (see also [4] for a related study). Similar results for N-particle dynamics are still open and we hope to be able to come back to this problem in the future.

The proof of Theorem 1 in [40] is built up on the previous works [30] and [39]. The main new ingredient is the following kinetic estimate.

Theorem 2 (Kinetic Estimate) *Let $\Psi_N(0)$ as in Theorem 1. Then for all $0 < \beta < 1/2$, all $\varepsilon > 0$ and all $t > 0$, we have*

$$\left\langle \Psi_N(t), \mathrm{d}\Gamma(Q(t)(1-\Delta)Q(t))\Psi_N(t)\right\rangle \le C_\varepsilon (N^{\beta+\varepsilon} + N^{3\beta-1}). \tag{7}$$

We can introduce the density matrix $\gamma^{(1)}_{\Psi_N(t)} : \mathfrak{H} \to \mathfrak{H}$ with kernel $\gamma^{(1)}_{\Psi_N(t)}(x,y) = \langle \Psi_N(t), a_y^* a_x \Psi_N(t)\rangle$ and rewrite (7) as

$$\mathrm{Tr}\Big(\sqrt{1-\Delta}Q(t)\gamma^{(1)}_{\Psi_N(t)}Q(t)\sqrt{1-\Delta}\Big) \le C_\varepsilon (N^{\beta+\varepsilon} + N^{3\beta-1}). \tag{8}$$

By the Cauchy-Schwarz inequality, (8) implies that for all $0 < \beta < 2/3$,

$$\lim_{N\to\infty} \mathrm{Tr}\left|\sqrt{1-\Delta}\Big(N^{-1}\gamma^{(1)}_{\Psi_N} - |u(t)\rangle\langle u(t)|\Big)\sqrt{1-\Delta}\right| = 0 \tag{9}$$

(see Sect. 3 for more details). In case $\beta = 0$, the approximation of the form (9) has been studied in [2, 36–38]. Note that (9) is stronger than the standard definition of the Bose-Einstein condensation

$$\lim_{N\to\infty} \mathrm{Tr}\left|N^{-1}\gamma^{(1)}_{\Psi_N} - |u(t)\rangle\langle u(t)|\right| = 0 \tag{10}$$

which has been studied by many authors; see [1, 6, 15, 16, 48] for some pioneer works (in these works, the convergence (10) was derived using the BBGKY hierarchy, a method that is less quantitative than our approach).

Note that when $\beta = 1$ (the Gross–Pitaevskii regime), the strong correlations between particles require a subtle correction: the nonlinear term $w_N * |u(t)|^2$ in Hartree equation (3) is replaced by $8\pi a|u(t)|^2$ with a the scattering length of w. This has been justified rigorously in the context of the Bose-Einstein condensation (10); see [32, 35, 43] for the ground state problem and [7, 17, 18, 44] for the dynamical problem. The norm approximation is completely open.

In the rest, we discuss Hartree and Bogoliubov equations in Sect. 2, and then go to the proofs of Theorems 2 and 1 in Sects. 3 and 4, respectively.

2 Effective Equations

We recall the well-posedness of Hartree equation from [23, Proposition 3.3 & Corollary 3.4].

Lemma 1 (Hartree Equation) *If $u(0,\cdot) \in H^2(\mathbb{R}^3)$, then Hartree equation (3) has a unique global solution $u \in C([0,\infty), H^2(\mathbb{R}^3)) \cap C^1((0,\infty), L^2(\mathbb{R}^3))$. Moreover, if $\|u(0,\cdot)\|_{W^{\ell,1}(\mathbb{R}^3)} \le C$ with ℓ sufficiently large, then*

$$\|u(t,\cdot)\|_{H^2} \le C, \quad \|\partial_t u(t,\cdot)\|_{L^2} \le C, \quad \|u(t,\cdot)\|_{L^\infty} + \|\partial_t u(t,\cdot)\|_{L^\infty} \le C(1+t)^{-3/2}.$$

As in [31, Sect. 2.3], any vector $\Psi \in \mathfrak{H}^N$ can be written uniquely as

$$\Psi = \sum_{n=0}^{N} u(t)^{\otimes(N-n)} \otimes_s \varphi_n = \sum_{n=0}^{N} \frac{(a^*(u(t)))^{N-n}}{\sqrt{(N-n)!}}\varphi_n$$

with $\varphi_n \in \mathfrak{H}_+(t)^n$. This gives rise to the unitary operator $U_N(t) : \mathfrak{H}^N \to \mathbb{1}^{\le N}\mathscr{F}_+(t)$

$$U_N(t)\Psi = \varphi_0 \oplus \varphi_1 \oplus \cdots \oplus \varphi_N.$$

Here $\mathbb{1}^{\le N}$ stands for the projection onto $\mathbb{C} \oplus \mathfrak{H} \oplus \cdots \oplus \mathfrak{H}^N$. Some fundamental properties of $U_N(t)$ can be found in [31, Proposition 4.2] and [30, Lemma 6].

Next, as in [30], we introduce $\Phi_N(t) := U_N(t)\Psi_N(t)$ and rewrite the Schrödinger equation as

$$i\partial_t \Phi_N(t) = \widetilde{H}_N(t)\Phi_N(t), \quad \Phi_N(0) = \mathbb{1}^{\le N}\Phi(0). \tag{11}$$

Here $\widetilde{H}_N(t) = \mathbb{1}^{\le N}\Big[\mathbb{H}(t) + \frac{1}{2}\sum_{j=0}^{4}(R_j + R_j^*)\Big]\mathbb{1}^{\le N}$ with

$$\begin{aligned}
R_0 &= \mathrm{d}\Gamma(Q(t)[w_N * |u(t)|^2 + \widetilde{K}_1(t) - \mu_N(t)]Q(t))\frac{1-\mathcal{N}}{N-1},\\
R_1 &= -2\frac{\mathcal{N}\sqrt{N-\mathcal{N}}}{N-1}a(Q(t)[w_N * |u(t)|^2]u(t)),\\
R_2 &= \iint K_2(t,x,y)a_x^* a_y^* \,\mathrm{d}x\,\mathrm{d}y\left(\frac{\sqrt{(N-\mathcal{N})(N-\mathcal{N}-1)}}{N-1} - 1\right),\\
R_3 &= \frac{\sqrt{N-\mathcal{N}}}{N-1}\iiiint (1\otimes Q(t)w_N Q(t)\otimes Q(t))(x,y;x',y')\times\\
&\qquad\qquad \times \overline{u(t,x)}a_y^* a_{x'} a_{y'}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}x'\,\mathrm{d}y',\\
R_4 &= \frac{1}{2(N-1)}\iiiint (Q(t)\otimes Q(t)w_N Q(t)\otimes Q(t))(x,y;x',y')\times\\
&\qquad\qquad \times a_x^* a_y^* a_{x'} a_{y'}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}x'\,\mathrm{d}y'.
\end{aligned}$$

(In R_0 and R_1 we write w_N for the function $w_N(x)$, while in R_3 and R_4 we write w_N for the two-body multiplication operator $w_N(x-y)$.)

The idea of Bogoliubov approximation is that when $N \to \infty$ all error terms R_j's are so small that we can ignore them and replace (11) by Bogoliubov equation (4). Some important properties of this equation are collected in the following

Lemma 2 (Bogoliubov Equation)

(i) If $\Phi(0)$ belongs to the quadratic form domain $\mathcal{Q}(\mathrm{d}\Gamma(1-\Delta))$, then Eq. (4) has a unique global solution in $\mathcal{Q}(\mathrm{d}\Gamma(1-\Delta))$. Moreover, the pair of density matrices $(\gamma_{\Phi(t)}, \alpha_{\Phi(t)})$ is the unique solution to

$$\begin{cases}
i\partial_t \gamma = h\gamma - \gamma h + K_2\alpha - \alpha^* K_2^*,\\
i\partial_t \alpha = h\alpha + \alpha h^{\mathrm{T}} + K_2 + K_2\gamma^{\mathrm{T}} + \gamma K_2,\\
\gamma(t=0) = \gamma_{\Phi(0)}, \quad \alpha(t=0) = \alpha_{\Phi(0)}.
\end{cases} \tag{12}$$

(ii) If we assume further that $\Phi(0)$ is a quasi-free state in $\mathscr{F}_+(0)$, then $\Phi(t)$ is a quasi-free state in $\mathscr{F}_+(t)$ for all $t > 0$ and

$$\langle \Phi(t), \mathcal{N}\Phi(t)\rangle \leq C\Big(\langle \Phi(0), \mathcal{N}\Phi(0)\rangle^2 + [\log(2+t)]^2\Big). \tag{13}$$

Recall that $\gamma_{\Phi(t)} : \mathfrak{H} \to \mathfrak{H}$, $\alpha_{\Phi(t)} : \overline{\mathfrak{H}} \equiv \mathfrak{H}^* \to \mathfrak{H}$ are operators with kernels $\gamma_{\Phi(t)}(x,y) = \langle \Phi(t), a_y^* a_x \Phi(t)\rangle$, $\alpha_{\Phi(t)}(x,y) = \langle \Phi(t), a_x a_y \Phi(t)\rangle$ and $K_2 : \overline{\mathfrak{H}} \equiv \mathfrak{H}^* \to \mathfrak{H}$ is an operator with kernel $K_2(t,x,y)$. Note that (12) is similar (but not identical) to the effective equations used in the Fock space setting in [23, 29].

Proof

(i) For existence and uniqueness of $\Phi(t)$, we refer to [30, Theorem 7]. To derive (12), we use (4) to compute

$$\begin{aligned}
&i\partial_t \gamma_{\Phi(t)}(x',y') = i\partial_t \langle \Phi(t), a_{y'}^* a_x \Phi(t)\rangle = \langle \Phi(t), [a_{y'}^* a_x, \mathbb{H}(t)]\Phi(t)\rangle \\
&= \iint h(t,x,y)\Big(\delta(x'-x)\gamma_{\Phi(t)}(y,y') - \delta(y'-y)\gamma_{\Phi(t)}(x',x)\Big)\,\mathrm{d}x\,\mathrm{d}y \\
&+ \frac{1}{2}\iint k(t,x,y)\Big(\delta(x'-x)\alpha^*_{\Phi(t)}(y,y') + \delta(x'-y)\alpha^*_{\Phi(t)}(y',x)\Big)\,\mathrm{d}x\,\mathrm{d}y \\
&- \frac{1}{2}\iint k^*(t,x,y)\Big(\delta(y'-y)\alpha_{\Phi(t)}(x,x') + \delta(y'-x)\alpha_{\Phi(t)}(y,x')\Big)\,\mathrm{d}x\,\mathrm{d}y \\
&= \Big(h(t)\gamma_{\Phi(t)} - \gamma_{\Phi(t)}h(t) + K_2(t)\alpha^*_{\Phi(t)} - \alpha_{\Phi(t)}K_2^*(t)\Big)(x',y')
\end{aligned}$$

This is the first equation in (12). The second equation is proved similarly.

(ii) Now we show that if $\Phi(0)$ is a quasi-free state, then $\Phi(t)$ is a quasi-free state for all $t > 0$. We will write $(\gamma,\alpha) = (\gamma_{\Phi(t)}, \alpha_{\Phi(t)})$ for short. Let us introduce

$$X := \gamma + \gamma^2 - \alpha\alpha^*, \quad Y := \gamma\alpha - \alpha\gamma^{\mathrm{T}}.$$

It is a general fact (see, e.g., [39, Lemma 8]) that $\Phi(t)$ is a quasi-free state if and only if $X(t) = 0$ and $Y(t) = 0$. In particular, we have $X(0) = 0$ and $Y(0) = 0$ by the assumption on $\Phi(0)$. Using (12) it is straightforward to see that

$$\begin{aligned}
&i\partial_t X = hX - Xh + kY^* - Yk^*, \\
&i\partial_t X^2 = (i\partial_t X)X + X(i\partial_t X) = hX^2 - X^2h + (K_2Y^* - YK_2^*)X + X(K_2Y^* - YK_2^*).
\end{aligned}$$

Then we take the trace and use $\mathrm{Tr}(hX^2 - X^2h) = 0$ (hX^2 and X^2h may be not trace class but we can introduce a cut-off; see [39] for details). We find that

$$\|X(t)\|_{\mathrm{HS}}^2 \leq 4\int_0^t \|K_2(s)\| \cdot \|X(s)\|_{\mathrm{HS}} \cdot \|Y(s)\|_{\mathrm{HS}} \, \mathrm{d}s$$

We also obtain a similar bound for $\|Y(t)\|_{\mathrm{HS}}$. Then summing these estimates and using the fact that $\|K_2(t)\|$ is bounded uniformly in time (see [40, Eq. (48)]) , we conclude by Grönwall's inequality that $X(t) = 0$, $Y(t) = 0$ for all $t > 0$.

A similar argument can be used to the uniqueness of solutions to (12).

To obtain (13), we first estimate $\|\alpha\|_{\mathrm{HS}}^2 + \|\gamma\|_{\mathrm{HS}}^2$ by a Grönwall-type inequality, and then use the identity $\|\alpha\|_{\mathrm{HS}}^2 = \mathrm{Tr}(\gamma + \gamma^2)$. We refer to [39] for details. □

3 Kinetic Bounds

In this section, we discuss Theorem 2. As mentioned, it is equivalent to (8) and in case $\beta < 2/3$ it implies (9). Let us explain the implication from (8) to (9) in more details. We will write $P(t) = |u(t)\rangle\langle u(t)|$ for short. We can decompose

$$\begin{aligned} N^{-1}\gamma^{(1)}_{\Psi_N(t)} - P(t) &= N^{-1}Q(t)\gamma^{(1)}_{\Psi_N(t)}Q(t) - N^{-1}\mathrm{Tr}\Big(Q(t)\gamma^{(1)}_{\Psi_N(t)}Q(t)\Big)P(t) \\ &\quad + N^{-1}Q(t)\gamma^{(1)}_{\Psi_N(t)}P(t) + N^{-1}P(t)\gamma^{(1)}_{\Psi_N(t)}Q(t) \end{aligned}$$

and use the triangle inequality of the trace norm to estimate

$$\begin{aligned} &\mathrm{Tr}\Big|\sqrt{1-\Delta}\Big(N^{-1}\gamma^{(1)}_{\Psi_N} - |u(t)\rangle\langle u(t)|\Big)\sqrt{1-\Delta}\Big| \\ &\leq N^{-1}\mathrm{Tr}\Big(\sqrt{1-\Delta}Q(t)\gamma^{(1)}_{\Psi_N(t)}Q(t)\sqrt{1-\Delta}\Big) + N^{-1}\mathrm{Tr}\Big(Q(t)\gamma^{(1)}_{\Psi_N(t)}Q(t)\Big)\|u(t,\cdot)\|_{H^1}^2 \\ &\quad + 2N^{-1}\mathrm{Tr}\Big|\sqrt{1-\Delta}Q(t)\gamma^{(1)}_{\Psi_N(t)}P(t)\sqrt{1-\Delta}\Big|. \end{aligned} \tag{14}$$

Using the Cauchy-Schwarz inequality (for Schatten norm)

$$\begin{aligned} &\mathrm{Tr}\left|(1-\Delta)^{1/2}Q(t)\gamma^{(1)}_{\Psi_N(t)}P(t)(1-\Delta)^{1/2}\right| \\ &\leq \left\|(1-\Delta)^{1/2}Q(t)\Big(\gamma^{(1)}_{\Psi_N(t)}\Big)^{1/2}\right\|_{\mathrm{HS}} \cdot \left\|\Big(\gamma^{(1)}_{\Psi_N(t)}\Big)^{1/2}\right\| \cdot \left\|P(t)(1-\Delta)^{1/2}\right\|_{\mathrm{HS}} \end{aligned}$$

we deduce from (8) and (14) that for all $\varepsilon > 0$,

$$\mathrm{Tr}\left|\sqrt{1-\Delta}\Big(N^{-1}\gamma^{(1)}_{\Psi_N} - |u(t)\rangle\langle u(t)|\Big)\sqrt{1-\Delta}\right| \le C_\varepsilon N^{a+\varepsilon} \tag{15}$$

where $a = \max\{\beta-1, (\beta-1)/2, 3\beta-2, (3\beta-2)/2\}$. If $\beta < 2/3$, then (9) holds.

Now we turn to another version of Theorem 2. From the definition $\Phi_N(t) = U_N(t)\Psi_N(t)$, we can check that $Q(t)\gamma^{(1)}_{\Psi_N}Q(t) = \gamma^{(1)}_{\Phi_N}$ (e.g. by using [31, Proposition 4.2]). Thus Theorem 2 is equivalent to

Theorem 3 (Kinetic Estimate) *Let $\Phi_N(t)$ be as in (11), with $\Phi(0)$ as in Theorem 1. Then for all $\varepsilon > 0$ and all $t > 0$, we have*

$$\big\langle \Phi_N(t), \mathrm{d}\Gamma(1-\Delta)\Phi_N(t)\big\rangle \le C_\varepsilon(N^{\beta+\varepsilon} + N^{3\beta-1+\varepsilon}). \tag{16}$$

Before proving Theorem 3, let us start with a simpler bound.

Lemma 3 (Bogoliubov Kinetic Bound) *Let $\Phi(t)$ be as in Theorem 1. Then*

$$\big\langle \Phi(t), \mathrm{d}\Gamma(1-\Delta)\Phi(t)\big\rangle \le C_\varepsilon N^{\beta+\varepsilon}, \quad \forall t > 0.$$

Proof For a general quadratic Hamiltonian, we have

$$\mathrm{d}\Gamma(H) + \frac{1}{2}\iint \Big(K(x,y)a^*_x a^*_y + \overline{K(x,y)}a_x a_y\Big)\,\mathrm{d}x\,\mathrm{d}y \ge -\frac{1}{2}\iint |(H_x^{-1/2}K(x,y)|^2\,\mathrm{d}x\,\mathrm{d}y.$$

This bound can be found in our recent joint work with Solovej [42, Lemma 9] (see also [11, Theorem 5.4] for a similar result). Combining this with the Sobolev-type estimate (see [40, Lemma 6])

$$\|(1-\Delta_x)^{-1/2}K_2(t,\cdot,\cdot)\|^2_{L^2} + \|(1-\Delta_x)^{-1/2}\partial_t K_2(t,\cdot,\cdot)\|^2_{L^2} \le C_\varepsilon(1+t)^{-3}N^{\beta+\varepsilon}$$

we obtain the quadratic form inequalities (see [40, Lemma 7])

$$\pm\Big(\mathbb{H}(t) + \mathrm{d}\Gamma(\Delta)\Big) \le \eta\mathrm{d}\Gamma(1-\Delta) + \frac{C_\varepsilon(\mathscr{N} + N^{\beta+\varepsilon})}{\eta(1+t)^3}, \tag{17}$$

$$\pm\partial_t\mathbb{H}(t) \le \eta\mathrm{d}\Gamma(1-\Delta) + \frac{C_\varepsilon(\mathscr{N} + N^{\beta+\varepsilon})}{\eta(1+t)^3}, \tag{18}$$

$$\pm i[\mathbb{H}(t), \mathscr{N}] \le \eta\mathrm{d}\Gamma(1-\Delta) + \frac{C_\varepsilon(\mathscr{N} + N^{\beta+\varepsilon})}{\eta(1+t)^3} \tag{19}$$

for all $\eta > 0$. On the other hand, from Bogoliubov equation (4), we have

$$\big\langle\Phi(t), \mathbb{H}(t)\Phi(t)\big\rangle - \big\langle\Phi(0), \mathbb{H}(0)\Phi(0)\big\rangle = \int_0^t \big\langle\Phi(s), \partial_s\mathbb{H}(s)\Phi(s)\big\rangle\,\mathrm{d}s. \tag{20}$$

Using (17) with $\eta = 1/2$ we have $\big\langle \Phi(0), \mathbb{H}(0)\Phi(0)\big\rangle \le C_\varepsilon N^{\beta+\varepsilon}$ and

$$\big\langle \Phi(t), \mathbb{H}(t)\Phi(t)\big\rangle \ge \frac{1}{2}\big\langle \Phi(t), \mathrm{d}\Gamma(1-\Delta)\Phi(t)\big\rangle - C_\varepsilon\Big(\big\langle \Phi(t), \mathcal{N}\Phi(t)\big\rangle + N^{\beta+\varepsilon}\Big)$$

Using (18) with $\eta = (1+t)^{-3/2}$ we get

$$\big\langle \Phi(t), \partial_t\mathbb{H}(t)\Phi(t)\big\rangle \le C_\varepsilon (1+t)^{-3/2}\Big(\big\langle \Phi(t), \mathrm{d}\Gamma(1-\Delta)\Phi(t)\big\rangle + N^{\beta+\varepsilon}\Big).$$

Thus (20) implies that

$$\begin{aligned}\big\langle \Phi(t), \mathrm{d}\Gamma(1-\Delta)\Phi(t)\big\rangle \le C_\varepsilon \int_0^t (1+s)^{-3/2}\big\langle \Phi(s), \mathrm{d}\Gamma(1-\Delta)\Phi(s)\big\rangle \,\mathrm{d}s \\ + C_\varepsilon\Big(\big\langle \Phi(t), \mathcal{N}\Phi(t)\big\rangle + N^{\beta+\varepsilon}\Big). \qquad (21)\end{aligned}$$

Similarly, we can estimate $\partial_t\langle \Phi(t), \mathcal{N}\Phi(t)\rangle$ by using Bogoliubov equation (4) and (19) with $\eta = (1+t)^{-3/2}$. Then we integrate the resulting bound and obtain

$$\langle \Phi(t), \mathcal{N}\Phi(t)\rangle \le C_\varepsilon \int_0^t (1+s)^{-3/2}\big\langle \Phi(s), \mathrm{d}\Gamma(1-\Delta)\Phi(s)\big\rangle \,\mathrm{d}s + C_\varepsilon N^{\beta+\varepsilon}.$$

Inserting the latter inequality into the right side of (21) we obtain

$$\big\langle \Phi(t), \mathrm{d}\Gamma(1-\Delta)\Phi(t)\big\rangle \le C_\varepsilon (1+s)^{-3/2}\int_0^t \big\langle \Phi(s), \mathrm{d}\Gamma(1-\Delta)\Phi(s)\big\rangle \,\mathrm{d}s + C_\varepsilon N^{\beta+\varepsilon}.$$

The desired result then follows from a Gronwall-type inequality. □

The proof of Theorem 3 is based on a similar argument. We will use the following estimates on the error terms R_j's in (11) (see [40, Lemmas 9, 11]).

Lemma 4 (Control of Error Terms) *Let R_j's be as in (11). Then we have the quadratic form estimates on $\mathbb{1}^{\le N}\mathscr{F}_+(t)$:*

$$\begin{aligned}\pm(R_j + R_j^*) \le& \eta\Big(R_4 + \frac{\mathcal{N}^2}{N}\Big) + \frac{C(1+\mathcal{N})}{\eta(1+t)^3}, \quad \forall \eta > 0,\ \forall j = 0,1,2,3,\\ 0 \le R_4 \le& CN^{3\beta-1}\mathcal{N}^2, \quad R_4 \le CN^{\beta-1}\mathrm{d}\Gamma(-\Delta)\mathcal{N},\\ \pm\partial_t(R_j + R_j^*) \le& \eta\Big(R_4 + \frac{\mathcal{N}^2}{N}\Big) + \frac{C(1+\mathcal{N})}{\eta(1+t)^3},\ \forall j = 0,1,2,3,4,\\ \pm i[(R_j + R_j^*), \mathcal{N}] \le& \eta\Big(R_4 + \frac{\mathcal{N}^2}{N}\Big) + \frac{C(1+\mathcal{N})}{\eta(1+t)^3},\ \forall j = 0,1,2,3,4.\end{aligned}$$

Now we are ready to provide

Proof (of Theorem 3) From (11) we have

$$\big\langle \Phi_N(t), \widetilde{H}_N(t)\Phi_N(t)\big\rangle - \big\langle \Phi_N(0), \widetilde{H}_N(0)\Phi_N(0)\big\rangle = \int_0^t \big\langle \Phi_N(s), \partial_s \widetilde{H}_N(s)\Phi_N(s)\big\rangle \,\mathrm{d}s. \tag{22}$$

Using (17) and Lemma 4, we can estimate

$$\begin{aligned}\big\langle \Phi_N(t), \widetilde{H}_N(t)\Phi_N(t)\big\rangle &\geq \frac{1}{2}\big\langle \Phi_N(t), (\mathrm{d}\Gamma(1-\Delta) + R_4)\Phi_N(t)\big\rangle \\ &\quad - C_\varepsilon\Big(N^{\beta+\varepsilon} + \big\langle \Phi_N(t), \mathcal{N}\Phi_N(t)\big\rangle\Big), \\ \big\langle \Phi_N(0), \widetilde{H}_N(0)\Phi_N(0)\big\rangle &\leq C_\varepsilon(N^{\beta+\varepsilon} + N^{3\beta-1+\varepsilon}).\end{aligned}$$

Here in the last inequality, we have used $R_4 \leq CN^{3\beta-1}\mathcal{N}^2$ (see Lemma 4) and a well-known moment estimate that holds for every quasi-free state Φ:

$$\Big\langle \Phi, (1+\mathcal{N})^s\Phi \Big\rangle \leq C_s \Big\langle \Phi, (1+\mathcal{N})\Phi\Big\rangle^s \tag{23}$$

where the constant C_s depends only on $s \in \mathbb{N}$ (see e.g. [39, Lemma 5]). Moreover, from (18) and Lemma 4 we obtain

$$\big\langle \Phi_N(t), \partial_t \widetilde{H}_N(t)\Phi_N(t)\big\rangle \leq C_\varepsilon (1+t)^{-3/2}\Big(\big\langle \Phi_N(t), (\mathrm{d}\Gamma(1-\Delta)+R_4)\Phi_N(t)\big\rangle + N^{\beta+\varepsilon}\Big).$$

Thus (22) implies that

$$\begin{aligned}\big\langle \Phi_N(t), (\mathrm{d}\Gamma(1-\Delta)+R_4)\Phi_N(t)\big\rangle &\leq C_\varepsilon \int_0^t \frac{\big\langle \Phi_N(s), (\mathrm{d}\Gamma(1-\Delta)+R_4)\Phi_N(s)\big\rangle}{(1+s)^{3/2}}\,\mathrm{d}s \\ &\quad + C_\varepsilon\Big(N^{\beta+\varepsilon} + N^{3\beta-1+\varepsilon} + \big\langle \Phi_N(t), \mathcal{N}\Phi_N(t)\big\rangle\Big).\end{aligned} \tag{24}$$

Next, we estimate $\partial_t\big\langle \Phi_N(t), \mathcal{N}\Phi_N(t)\big\rangle$ by using (11), (19) and the last inequality in Lemma 4. Then we integrate the resulting bound to get

$$\langle \Phi(t), \mathcal{N}\Phi(t)\rangle \leq C_\varepsilon \int_0^t (1+s)^{-3/2}\big\langle \Phi_N(s), (\mathrm{d}\Gamma(1-\Delta)+R_4)\Phi_N(s)\big\rangle\,\mathrm{d}s + C_\varepsilon N^{\beta+\varepsilon}.$$

Substituting the latter estimate into (24), we find that

$$\begin{aligned}&\big\langle \Phi_N(t), (\mathrm{d}\Gamma(1-\Delta)+R_4)\Phi_N(t)\big\rangle \\ &\leq C_\varepsilon \int_0^t \frac{\big\langle \Phi_N(s), (\mathrm{d}\Gamma(1-\Delta)+R_4)\Phi_N(s)\big\rangle}{(1+s)^{3/2}}\,\mathrm{d}s + C_\varepsilon(N^{\beta+\varepsilon} + N^{3\beta-1+\varepsilon}).\end{aligned}$$

By a Gronwall-type inequality, we conclude that

$$\big\langle \Phi_N(t), (\mathrm{d}\Gamma(1-\Delta) + R_4)\Phi_N(t)\big\rangle \le C_\varepsilon (N^{\beta+\varepsilon} + N^{3\beta-1+\varepsilon}).$$

Since $R_4 \ge 0$, the desired kinetic estimate follows. □

4 Norm Approximation

Proof (of Theorem 1) **Step 1.** The desired estimate (6) is

$$\|\Psi_N(t) - U_N(t)^* \mathbb{1}^{\le N}\Phi(t)\|^2_{\mathfrak{H}^N} \le C_\varepsilon (1+t)^{1+\varepsilon} N^{(2\beta+\varepsilon-1)/2}, \quad \forall \varepsilon > 0.$$

Since $\Phi(t) = U_N(t)\Psi_N(t)$ and $U_N(t) : \mathfrak{H}^N \to \mathbb{1}^{\le N}\mathscr{F}_+(t)$ is a unitary operator,

$$\|\Psi_N(t) - U_N(t)^*\mathbb{1}^{\le N}\Phi(t)\|_{\mathfrak{H}^N} = \|U_N(t)\Psi_N(t) - \mathbb{1}^{\le N}\Phi(t)\| \le \|\Phi_N(t) - \Phi(t)\|.$$

It remains to bound $\|\Phi_N(t) - \Phi(t)\|$. Using Eqs. (4) and (11), we can write

$$\begin{aligned} \partial_t \|\Phi_N(t) - \Phi(t)\|^2 &= 2\Re \left\langle i\Phi_N(t), (\widetilde{H}_N(t) - \mathbb{H}(t))\Phi(t)\right\rangle \qquad (25) \\ &= \sum_{j=0}^{4} \Re\big\langle i\Phi_N(t), (R_j + R_j^*)\mathbb{1}^{\le N}\Phi(t)\big\rangle - 2\Re\left\langle i\Phi_N(t), \mathbb{H}\mathbb{1}^{>N}\Phi(t)\right\rangle \end{aligned}$$

where $\mathbb{1}^{>N} := \mathbb{1} - \mathbb{1}^{\le N}$. Next, we will estimate the right side of (25).
Step 2. To bound the last term of (25), we use $\Phi_N(t) \in \mathbb{1}^{\le N}\mathscr{F}_+(t)$ to write

$$\big\langle \Phi_N(t), \mathbb{H}\mathbb{1}^{>N}\Phi(t)\big\rangle = \big\langle \Phi_N(t), (\mathbb{H} - \mathrm{d}\Gamma(h))\mathbb{1}^{>N}\Phi(t)\big\rangle.$$

As in the proof of Lemma 3, we can show that

$$\pm(\mathbb{H} - \mathrm{d}\Gamma(h)) \le C(\mathscr{N} + N^{3\beta}).$$

It is a general fact that if $\pm B \le A$ as quadratic forms, then we have the Cauchy-Schwarz type inequality $|\langle f, Bg\rangle| \le 3\langle f, Af\rangle^{1/2}\langle g, Ag\rangle^{1/2}$. Consequently,

$$\begin{aligned} &\big|\big\langle \Phi_N(t), (\mathbb{H} - \mathrm{d}\Gamma(h))\mathbb{1}^{>N}\Phi(t)\big\rangle\big| \\ &\le 3\big\langle \Phi_N(t), (\mathscr{N} + N^{3\beta})\Phi_N(t)\big\rangle^{1/2}\big\langle \mathbb{1}^{>N}\Phi(t), (\mathscr{N} + N^{3\beta})\mathbb{1}^{>N}\Phi(t)\big\rangle^{1/2} \\ &\le 3(N + N^{3\beta})^{1/2}\big\rangle^{1/2}\big\langle \mathbb{1}^{>N}\Phi(t), (\mathscr{N} + N^{3\beta})\mathscr{N}^s N^{-s}\mathbb{1}^{>N}\Phi(t)\big\rangle^{1/2} \end{aligned}$$

for all $s \geq 1$. The term $\langle \Phi(t), \mathcal{N}^s \Phi(t)\rangle$ can be bounded by (23) and the bound on $\langle \Phi(t), \mathcal{N} \Phi(t)\rangle$ in Lemma 2. We can choose s large enough (but fixed) and obtain

$$\left|\left\langle \Phi_N(t), \mathbb{H}\mathbb{1}^{>N}\Phi(t)\right\rangle\right| \leq C_\varepsilon (1+t)^\varepsilon N^{-1}. \tag{26}$$

Step 3. To control the first term on the right side of (25), we have to introduce a cut-off on the number of particles. Since there are at most 2 creation or annihilation operators in the expressions of R_j's, we can write

$$\begin{aligned}\left\langle \Phi_N(t), (R_j + R_j^*)\mathbb{1}^{\leq N}\Phi(t)\right\rangle &= \left\langle \mathbb{1}^{\leq M}\Phi_N(t), (R_j + R_j^*)\mathbb{1}^{\leq M+2}\Phi(t)\right\rangle \\ &\quad + \left\langle \mathbb{1}^{>M}\Phi_N(t), (R_j + R_j^*)\mathbb{1}^{\leq N}\mathbb{1}^{>M-2}\Phi(t)\right\rangle\end{aligned}$$

for all $4 < M < N-2$. Then we estimate each term on the right side by Lemma 4 and the Cauchy-Schwarz type inequality as in Step 2. We obtain

$$\left|\left\langle \Phi_N(t), (R_j + R_j^*)\mathbb{1}^{\leq N}\Phi(t)\right\rangle\right| \leq C(E_1 + E_2) \tag{27}$$

where

$$\begin{aligned}E_1 = \inf_{\eta>0} &\left\langle \mathbb{1}^{\leq M}\Phi_N(t), \left((1+\eta)R_4 + \eta\frac{\mathcal{N}^2}{N} + \frac{1+\mathcal{N}}{\eta(1+t)^3}\right)\mathbb{1}^{\leq M}\Phi_N(t)\right\rangle^{1/2} \\ &\times \left\langle \mathbb{1}^{\leq M+2}\Phi(t), \left((1+\eta)R_4 + \eta\frac{\mathcal{N}^2}{N} + \frac{1+\mathcal{N}}{\eta(1+t)^3}\right)\mathbb{1}^{\leq M+2}\Phi(t)\right\rangle^{1/2}, \\ E_2 = \inf_{\eta>0} &\left\langle \mathbb{1}^{>M}\Phi_N(t), \left((1+\eta)R_4 + \eta\frac{\mathcal{N}^2}{N} + \frac{1+\mathcal{N}}{\eta(1+t)^3}\right)\mathbb{1}^{>M}\Phi_N(t)\right\rangle^{1/2} \\ &\times \left\langle \mathbb{1}^{>M-2}\Phi(t), \left((1+\eta)R_4 + \eta\frac{\mathcal{N}^2}{N} + \frac{1+\mathcal{N}}{\eta(1+t)^3}\right)\mathbb{1}^{>M-2}\Phi(t)\right\rangle^{1/2}.\end{aligned}$$

To bound E_1, we use

$$\mathbb{1}^{\leq M}R_4 \leq CN^{\beta-1}\mathbb{1}^{\leq M}\mathcal{N}\mathrm{d}\Gamma(-\Delta) \leq CN^{\beta-1}M\mathrm{d}\Gamma(-\Delta)$$

(see Lemma 4) together with the kinetic estimate in Theorem 3, and then optimize over $\eta > 0$. We get

$$E_1 \leq C_\varepsilon\left(MN^{(2\beta+\varepsilon-1)/2} + M^{3/2}N^{-1/2}\right).$$

(The error term $N^{3\beta-1+\varepsilon}$ in Theorem 3 is absorbed by $N^{\beta+\varepsilon}$ when $\beta < 1/2$.)

The bound on E_2 is obtained using the argument in Step 2 and reads

$$E_2 \leq C_{\varepsilon,s}N^{3\beta+1}M^{1-s/2}N^{s\varepsilon}[\log(2+t)]^s.$$

In summary, from (27) it follows that

$$\left|\left\langle \Phi_N(t), (R_j + R_j^*)\mathbb{1}^{\leq N}\Phi(t)\right\rangle\right| \leq C_\varepsilon\Big(MN^{(2\beta+\varepsilon-1)/2} + M^{3/2}N^{-1/2}\Big) + C_{\varepsilon,s}N^{3\beta+1}M^{1-s/2}N^{s\varepsilon}[\log(2+t)]^s$$

for all $4 < M < N-2$ and $s \geq 2$. We can choose $M = N^{3\varepsilon}$ and $s = s(\varepsilon)$ sufficiently large (e.g. $s \geq 6(1+\beta+\varepsilon)/\varepsilon$) to obtain

$$\left|\left\langle \Phi_N(t), (R_j + R_j^*)\mathbb{1}^{\leq N}\Phi(t)\right\rangle\right| \leq C_\varepsilon\Big(N^{(2\beta+9\varepsilon-1)/2} + N^{-1}(1+t)^\varepsilon\Big). \tag{28}$$

Step 4. Inserting (26) and (28) into (25), we find that

$$\partial_t\|\Phi_N(t) - \Phi(t)\|^2 \leq C_\varepsilon\Big(N^{(2\beta+9\varepsilon-1)/2} + N^{-1}(1+t)^\varepsilon\Big).$$

Integrating over t and using

$$\|\Phi_N(0) - \Phi(0)\|^2 = \langle \Phi(0), \mathbb{1}^{>N}\Phi(0)\rangle \leq N^{-1}\langle \Phi(0), \mathcal{N}\Phi(0)\rangle \leq C_\varepsilon N^{\varepsilon-1}.$$

we obtain

$$\|\Phi_N(t) - \Phi(t)\|^2 \leq C_\varepsilon(1+t)^{1+\varepsilon}N^{(2\beta+9\varepsilon-1)/2}$$

for all $\varepsilon > 0$. This leads to the desired estimate (6), as explained in Step 1. □

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Effective Non-linear Dynamics of Binary Condensates and Open Problems

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Abstract We report on a recent result concerning the effective dynamics for a mixture of Bose-Einstein condensates, a class of systems much studied in physics and receiving a large amount of attention in the recent literature in mathematical physics; for such models, the effective dynamics is described by a coupled system of non-linear Schödinger equations. After reviewing and commenting our proof in the mean-field regime from a previous paper, we collect the main details needed to obtain the rigorous derivation of the effective dynamics in the Gross-Pitaevskii scaling limit.

Keywords Coupled nonlinear Schrödinger system • Cubic NLS • Effective non-linear evolution equations • Gross-Pitaevskii scaling • Manybody quantum dynamics • Mean-field regime • Mixture condensates • Partial trace • Reduced density matrix

1 Introduction

Bose-Einstein condensation is the physical phenomenon according to which a macroscopic number of bosons collapse onto the same quantum state. This was first predicted theoretically in the 1920s and then widely studied both in physics and mathematics in the later decades; the topic received a further strong boost since the mid 1990s, when the first condensates were produced in experiments.

Mathematically, to a system of N identical bosons is associated the Hilbert space $L^2(\mathbb{R}^3)^{\otimes_{\mathrm{sym}} N}$ and states are positive trace-class operators γ_N on such space, with unit trace. The notion of condensation is appropriately described in terms of the corresponding one-body reduced density matrix, or one-body marginal,

$$\gamma_N^{(1)} = \mathrm{Tr}_{N-1}\gamma_N, \tag{1}$$

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A. Michelangeli, G. Dell'Antonio (eds.), *Advances in Quantum Mechanics*,
Springer INdAM Series 18, DOI 10.1007/978-3-319-58904-6_14

where the degrees of freedom 2 to N are traced out; the operation Tr_{N-1} in (1) is called the partial trace. Thus, given a N-body density matrix γ_N of the system, and a pure state $u \in L^2(\mathbb{R}^3)$, one says that γ_N exhibits complete asymptotic condensation on the condensate wave-function u if

$$\lim_{N\to\infty} \gamma_N^{(1)} = |u\rangle\langle u|. \tag{2}$$

Since the limit in (2) is a rank-one projection, weak convergence implies trace-norm convergence, and thus, the limit can be considered in any of such topologies.

Within this framework, a problem naturally arising is the proof of persistence of condensation under the dynamics generated by some many-body Hamiltonian. Thus, given a time-evolution governed by H_N, and the flow

$$\gamma_N \mapsto \gamma_{N,t} = e^{-\mathrm{i}tH_N}\gamma_N e^{\mathrm{i}tH_N},$$

one would like to prove that

$$\gamma_N^{(1)} \simeq |u_0\rangle\langle u_0| \quad \Rightarrow \quad \gamma_{N,t}^{(1)} \simeq |u_t\rangle\langle u_t|. \tag{3}$$

The interest in a result like (3) is manifest: a large system is well approximated by a single-particle orbital, an object much more manageable in computations and informative when one-body observables are considered. The price to pay is that in the limit the interparticle interactions result in a non-linearity, or self-interaction term; hence, a typical equation for u_t is

$$\mathrm{i}\partial_t u_t = -\Delta u_t + \mathscr{N}(u_t)u_t,$$

where, as said, $\mathscr{N}(.)$ accounts for the effective two-body potential via a cubic self-interaction. We refer to the review [3] for a comprehensive outlook on the problem. It has to be remarked that this class of problems has involved many different techniques, with tools from operator theory, measure theory and kinetic theory.

2 Two-Component Condensates

A consistent part of both theoretical and experimental studies on Bose-Einstein condensation is devoted to systems in which two (or more) components interact; such systems are usually referred to as two-component condensates (respectively multi-component condensates). This can be attained in multiple ways: either by considering bosons occupying different hyperfine spin states [16, 23] (spinor condensates) or by considering different atomic species [15] (mixture condensates); in the case of different spin states, one can also account for transitions between the two components, for example by turning on an external magnetic field or a spin-spin interaction (this is discussed in Sect. 5). Physical evidence suggests that the dynamics of a multi-component condensate is governed by a coupled system of non-linear Schrödinger equations (see [22, Sect. 21]), the unknowns being the condensate wave-functions of each component.

In this work we consider the case of the mixture condensate, namely a system consisting of N_1 identical bosons of some atomic species A and N_2 identical bosons of some (different) species B; the Hilbert space of such system is

$$\mathscr{H}_{N_1,N_2} = L^2_{\text{sym}}(\mathbb{R}^{3N_1}, dx_1 \dots dx_{N_1}) \otimes L^2_{\text{sym}}(\mathbb{R}^{3N_1}, dy_1 \dots dy_{N_2}). \tag{4}$$

We want to consider states of such system in which condensation is present in each component: this can be monitored by means of a *"double" reduced density matrix*. For each state γ_{N_1,N_2} of the system, we define the trace-class operator

$$\gamma^{(1,1)}_{N_1,N_2} = \text{Tr}_{N_1-1} \otimes \text{Tr}_{N_2-1} \gamma_{N_1,N_2}, \tag{5}$$

acting on the space $L^2(\mathbb{R}^3, dx) \otimes L^2(\mathbb{R}^3, dy)$ of one particle of type A and one of type B.

In this setting, one can extend the notion of condensation, namely, one says γ_{N_1,N_2} exhibits complete condensation in both components, with condensate functions u and v, if

$$\lim_{\substack{N_1\to\infty \\ N_2\to\infty}} \gamma^{(1,1)}_{N_1,N_2} = |u \otimes v\rangle\langle u \otimes v| = |u\rangle\langle u| \otimes |v\rangle\langle v|. \tag{6}$$

In analogy to the one-component case, it is of interest to investigate the persistence of condensation simultaneously in each component. Of course one has to specify a Hamiltonian generating the time-evolution; moreover, since at the moment no result is attainable in a genuine thermodynamic limit of large system, the Hamiltonian must be chosen together with a scaling prescription that mimics the true limit [3, 10].

2.1 Mean-Field Regime

For the multi-component system built in Sect. 2, we define the three-dimensional mean-field Hamiltonian

$$\begin{aligned} H_{N_1,N_2} &= \sum_{i=1}^{N_1}(-\Delta_{x_i}) + \frac{1}{N_1}\sum_{i<j}^{N_1} V_1(x_i - x_j) \\ &\quad + \sum_{r=1}^{N_2}(-\Delta_{y_r}) + \frac{1}{N_2}\sum_{r<s}^{N_2} V_2(y_r - y_s) \\ &\quad + \frac{1}{N_1+N_2}\sum_{i=1}^{N_1}\sum_{r=1}^{N_2} V_{12}(x_i - y_r), \end{aligned} \tag{7}$$

where the variables $x_1, \dots x_{N_1}, y_1 \dots y_{N_2}$ are referred to the ones in Eq. (4).

Throughout this paper, we will consider the case in which N_1 and N_2 scale in such a way that their ratio is asymptotically constant, namely there exist constants $c_1, c_2 > 0$ such that

$$c_i = \lim_{\substack{N_1 \to \infty \\ N_2 \to \infty}} \frac{N_i}{N_1 + N_2}, \quad i = 1, 2. \tag{8}$$

For simplicity of presentation, we assume that (8) holds identically for every fixed N_1 and N_2, and not only in the limit; this stronger assumption could easily be removed. Under such assumptions, it is easy to see that our choice of the mean-field pre-factors N_1^{-1}, N_2^{-1}, $(N_1 + N_2)^{-1}$ ensures all terms in (7) to remain of the same order $O(N_1 + N_2)$. Of course, one could argue that many other choices would ensure this behavior, for example a common $(N_1 N_2)^{-1/2}$ factor; the reader can refer to Sect. 4 in [12] for a discussion of why the choice in (7) is *the* physically relevant mean-field scaling.

Our result is the proof of persistence of condensation under the dynamics generated by (7), namely

$$\gamma^{(1,1)}_{N_1,N_2}(0) \;\simeq\; |u_0 \otimes v_0\rangle\langle u_0 \otimes v_0| \quad \Rightarrow \quad \gamma^{(1,1)}_{N_1,N_2}(t) \simeq\; |u_t \otimes v_t\rangle\langle u_t \otimes v_t|, \tag{9}$$

where (u_t, v_t) solves the initial value problem

$$\begin{aligned} \mathrm{i}\partial_t u_t &= -\Delta u_t + (V_1 * |u_t|^2)u_t + c_2(V_{12} * |v_t|^2)u_t \\ \mathrm{i}\partial_t v_t &= -\Delta v_t + (V_2 * |v_t|^2)v_t + c_1(V_{12} * |u_t|^2)v_t, \end{aligned} \tag{10}$$

with initial datum (u_0, v_0).

Let us now state the assumptions on V_j and (u_0, v_0) under which it is possible to prove (9).

- (A1) The potentials $V_j, j \in \{1, 2, 12\}$ are real-valued, even, and such that

$$\begin{aligned} \|V_j * |\phi|^2\|_\infty &\lesssim \|\phi\|^2_{H^1} \qquad \forall \phi \in H^1(\mathbb{R}^3) \qquad j = 1, 2, 12 \\ \|V_j^2 * |\phi|^2\|_\infty &\lesssim \|\phi\|^2_{H^1} \qquad \forall \phi \in H^1(\mathbb{R}^3) \qquad j = 1, 2, 12. \end{aligned} \tag{11}$$

- (A2) The initial data for the system (10) are $u(0) = u_0$ and $v(0) = v_0$ for given functions $u_0, v_0 \in H^1(\mathbb{R}^3)$ with $\|u_0\|_2 = \|v_0\|_2 = 1$. By general theory, this is enough to have a unique global-in-time solution

$$(u_t, v_t) \;\in\; C(\mathbb{R}, H^1(\mathbb{R}^3) \oplus H^1(\mathbb{R}^3)) \cap C^1(\mathbb{R}, H^{-1}(\mathbb{R}^3) \oplus H^{-1}(\mathbb{R}^3)). \tag{12}$$

- (A3) The many-body initial datum is $\Psi_{N_1,N_2} \in \mathscr{D}[H_{N_1,N_2}] \cap \mathscr{H}_{N_1,N_2,\mathrm{sym}}$ with $\|\Psi_{N_1,N_2}\|_2 = 1$.

Let $\Psi_{N_1,N_2}(t) := e^{-\mathrm{i}tH_{N_1,N_2}}\Psi_{N_1,N_2}$ be the unique solution in $C(\mathbb{R}, \mathscr{D}[H_{N_1,N_2}] \cap \mathscr{H}_{N_1,N_2,\mathrm{sym}})$ to the many-body Schrödinger equation

$$\mathrm{i}\partial_t \Psi_{N_1,N_2}(t) \;=\; H_{N_1,N_2}\Psi_{N_1,N_2}(t)\,, \qquad \Psi_{N_1,N_2}(0) = \Psi_{N_1,N_2}\,, \tag{13}$$

and let (u_t, v_t) be the unique solution to the system of coupled NLS (10) as in (12). Our main result in the mean-field regime is the following Theorem.

Theorem 1 ([12]) *Consider a two-species bosonic system under assumptions (A1)–(A3) above. Let $\gamma^{(1,1)}_{N_1,N_2}(t)$ be the double reduced density matrix associated with $\Psi_{N_1,N_2}(t)$, given by (5), and define*

$$\alpha^{(1,1)}_{N_1,N_2}(t) \;:=\; 1 - \big\langle u_t \otimes v_t\,,\; \gamma^{(1,1)}_{N_1,N_2}(t)\; u_t \otimes v_t \big\rangle\,. \tag{14}$$

Then

$$\alpha^{(1,1)}_{N_1,N_2}(t) \;\leqslant\; \left(\alpha^{(1,1)}_{N_1,N_2}(0) + \frac{1}{N_1+N_2}\right) e^{f(t)}, \tag{15}$$

where f does not depend on N.

Corollary 1 ([12]) *In the same hypothesis of Theorem 1, if*

$$\lim_{\substack{N_1\to\infty\\N_2\to\infty}} \gamma^{(1,1)}_{N_1,N_2}(0) = \; |u_0 \otimes v_0\rangle\langle u_0 \otimes v_0|,$$

in trace norm, then

$$\lim_{\substack{N_1\to\infty\\N_2\to\infty}} \gamma^{(1,1)}_{N_1,N_2}(t) = \; |u_t \otimes v_t\rangle\langle u_t \otimes v_t|,$$

again in trace norm.

We show here the immediate proof of Corollary 1, postponing to Sect. 3 a sketch of the proof of Theorem 1,

Proof (Corollary 1) The thesis follows from (15) using the chain of inequalities (see [12] Eq. (3.7) or [11])

$$\alpha^{(1,1)}_{N_1,N_2}(t) \leqslant \mathrm{Tr}\Big|\gamma^{(1,1)}_{N_1,N_2}(t) - |u_t \otimes v_t\rangle\langle u_t \otimes v_t|\Big| \leqslant C\sqrt{\alpha^{(1,1)}_{N_1,N_2}(t)}. \tag{16}$$

A few remarks on the results we stated are in order.

Remark 1 Assumption (A1) covers, by Hardy inequality, the physically relevant case of Coulomb singularities $|x|^{-1}$.

Remark 2 To keep the exposition short and self-contained, we limited the class of Hamiltonians for which a result like Theorem 1 holds; in particular, one could deal with several meaningful generalizations of the one-body operator $-\Delta$, as for example the magnetic Laplacian with external potential $-\Delta_A + U(x)$, or its semi-relativistic counterpart $(1-\Delta_A)^{1/2} + U(x)$, where $\Delta_A := (\nabla - iA)^2$.

Remark 3 The second bound in (16) is not sharp: indeed, one could adapt a recent result [14] and obtain convergence in trace norm *with the same rate as the convergence of* $\alpha^{(1,1)}_{N_1,N_2}$. This, by (15), implies that the total rate is the worst among the rates of $\alpha^{(1,1)}_{N_1,N_2}(0)$ and of $(N_1+N_2)^{-1}$.

The functional $\alpha^{(1,1)}_{N_1,N_2}(t)$ is a two-component generalization of the one-component functional

$$\alpha_N(t) := 1 - \langle \psi_N(t), p_1(t)\psi_N(t)\rangle,$$

where

$$p_1(t) := |u_t\rangle_1\langle u_t|_1 \tag{17}$$

is the projection onto the condensate wave-function in the variable x_1; for later convenience we also define the orthogonal complement to p as

$$q_1(t) := \mathbb{1} - p_1(t). \tag{18}$$

Such a construction is the starting point of the so-called "counting" method introduced by Pickl in [20] and by Knowles and Pickl in [9]. In those works, $\alpha_N(t)$ is used to prove trace-norm convergence with a quantitative rate for a wide class of potentials in the single component case.

The meaning of Eq. (16) (and of its one-component counterpart, see Lemma 2.3 in [9]) is that $\alpha^{(1,1)}_{N_1,N_2}$ is a convenient indicator of condensation, namely its convergence to zero is tantamount as the convergence in trace norm to the condensate wave-function. In our two-component case, one could also argue that condensation can also be expressed in terms of one-component reduced density matrices, which can be defined as

$$\gamma^{(1,0)}_{N_1,N_2} = \mathrm{Tr}_{N_1-1} \otimes \mathrm{Tr}_{N_2}\gamma_{N_1,N_2}, \qquad \gamma^{(0,1)}_{N_1,N_2} = \mathrm{Tr}_{N_1} \otimes \mathrm{Tr}_{N_2-1}\gamma_{N_1,N_2}. \tag{19}$$

The control of condensation by means of both $\gamma^{(1,0)}_{N_1,N_2}$ and $\gamma^{(0,1)}_{N_1,N_2}$ has been addressed by Heil [6] (we also refer to [1] for a more recent work); in Lemma 3.1 in [12] we establish the bound

$$\begin{aligned} \max\left\{1 - \langle u, \gamma^{(1,0)}_{N_1,N_2} u\rangle\,,\, 1 - \langle v, \gamma^{(0,1)}_{N_1,N_2} v\rangle\right\} &\leqslant 1 - \langle u\otimes v, \gamma^{(1,1)}_{N_1,N_2} u\otimes v\rangle \\ &\leqslant (1 - \langle u, \gamma^{(1,0)}_{N_1,N_2} u\rangle) + (1 - \langle v, \gamma^{(0,1)}_{N_1,N_2} v\rangle), \end{aligned} \tag{20}$$

which shows that our collective indicator $\gamma^{(1,1)}_{N_1,N_2}$ covers (and is in fact equivalent to) such a control.

2.2 Gross-Pitaevskii Regime

The mean-field result stated above can be extended to the more interesting and realistic Gross-Pitaevskii regime we describe in the following; in its essence, what we report already stems from the work [12]. Nonetheless, we state here the result and present the main steps of the proof, in order to provide an explicit reference.

Consider the two-component Hamiltonian

$$\begin{aligned} H_{N_1,N_2} \;=\; & \sum_{i=1}^{N_1}(-\Delta_{x_i}) + N_1^2 \sum_{i<j}^{N_1} V_1(N_1(x_i - x_j)) \\ & + \sum_{r=1}^{N_2}(-\Delta_{y_r}) + N_2^2 \sum_{r<s}^{N_2} V_2(N_2(y_r - y_s)) \\ & + (N_1+N_2)^2 \sum_{i=1}^{N_1}\sum_{r=1}^{N_2} V_{12}((N_1+N_2)(x_i - y_r)), \end{aligned} \tag{21}$$

where now the potentials are rescaled according to the Gross-Pitaevskii scaling. This implies very strong ($\sim N^2$) but rare interactions, since particles interact only when their distances are of order N^{-1}, and this makes the regime quite different from the mean field in Sect. 2.1: whereas in mean field each particle only feels the average density of the whole gas, in the Gross-Pitaevskii regime interactions are very strong and effective only on short spatial scales. For this reason, this scaling is a much more realistic approximation for a gas in a zero temperature and high dilution regime.

One can prove a statement similar to Theorem 1 also in this case, but with an amount of modifications. Indeed, now the limit (9) holds for (u_t, v_t) solutions to the *local* system of NLS

$$\begin{aligned} \mathrm{i}\partial_t u_t &= -\Delta u_t + 8\pi a_1 |u_t|^2 u_t + c_2\, 8\pi a_{12} |v_t|^2 u_t \\ \mathrm{i}\partial_t v_t &= -\Delta v_t + 8\pi a_2 |v_t|^2 v_t + c_1\, 8\pi a_{12} |u_t|^2 v_t, \end{aligned} \tag{22}$$

where, for $j \in \{1, 2, 12\}$, a_j is the s-wave scattering length of V_j.

Since, to treat the Gross-Pitaevskii case, one also has to take into account energy comparisons between many-body and effective dynamics, we define the following two functionals: the many-body energy functional

$$\mathscr{E}_{N_1,N_2}(\Psi_{N_1,N_2}) := \frac{1}{N_1+N_2}\langle \Psi_{N_1,N_2}, H_{N_1,N_2}\Psi_{N_1,N_2}\rangle, \tag{23}$$

and the Gross-Pitaevskii energy

$$\begin{aligned}\mathscr{E}^{GP}(u,v) :=& \langle u, -\Delta u\rangle + \langle v, -\Delta v\rangle + 4\pi a_1 \langle u, |u|^2 u\rangle \\ &+ 4\pi a_2 \langle v, |v|^2 v\rangle + 8\pi a_{12}\langle u, |v|^2 u\rangle.\end{aligned} \tag{24}$$

We suppose the following on the potential and on the initial data.

- (B1) The potentials V_α, $\alpha \in \{1, 2, 12\}$ are positive, spherically symmetric, compactly supported, L^∞-functions.
- (B2) The initial data for the system (10) are $u(0) = u_0$ and $v(0) = v_0$ for given functions $u_0, v_0 \in L^2(\mathbb{R}^3)$ with $\|u_0\|_2 = \|v_0\|_2 = 1$ chosen such that the solution belongs to

$$L^\infty\Big(\mathbb{R}, H^2(\mathbb{R}^3) \oplus H^2(\mathbb{R}^3)\Big).$$

- (B3) The many-body initial datum is $\Psi_{N_1,N_2} \in \mathscr{D}[H_{N_1,N_2}] \cap \mathscr{H}_{N_1,N_2,\mathrm{sym}}$ with $\|\Psi_{N_1,N_2}\|_2 = 1$ and

$$\lim_{\substack{N_1\to\infty\\N_2\to\infty}} \gamma^{(1,1)}_{N_1,N_2} = |u_0 \otimes v_0\rangle\langle u_0 \otimes v_0|.$$

- (B4) The sequence Ψ_{N_1,N_2} satisfies

$$\lim_{\substack{N_1\to\infty\\N_2\to\infty}} \mathscr{E}_{N_1,N_2}(\Psi_{N_1,N_2}) = \mathscr{E}^{GP}(u_0, v_0).$$

Here is our main result.

Theorem 2 *Consider a two-species bosonic system under assumptions (B1)–(B4) above. Let $\gamma^{(1,1)}_{N_1,N_2}(t)$ be the double reduced density matrix associated with $\Psi_{N_1,N_2}(t)$, given by (5). Then*

$$\lim_{\substack{N_1\to\infty\\N_2\to\infty}} \gamma^{(1,1)}_{N_1,N_2}(t) = |u_t \otimes v_t\rangle\langle u_t \otimes v_t|, \tag{25}$$

and

$$\lim_{\substack{N_1\to\infty\\N_2\to\infty}} \mathscr{E}_{N_1,N_2}(\Psi_{N_1,N_2}(t)) = \mathscr{E}^{GP}(u_t, v_t), \tag{26}$$

where (u_t, v_t) are solutions of (22) with initial data (u_0, v_0).

Remark 4 A generalization of the technique used in the proof allows one to cover also the case of one-body Hamiltonians more general than $-\Delta$. This has been pointed out in the single component case in Remark 2.1 in [21]; we refer the reader to [18] for a more detailed analysis of what is needed in order to adapt the argument to the relevant case of the magnetic Laplacian $\Delta_A = (\nabla - iA)^2$.

Remark 5 Assumption (B1) on the potential is crucial in this formalism; with different techniques (see [2]) it is possible to consider potentials with some singularity and unbounded support. Conversely, the removal of the positivity condition is an important open problem in the subject; in [19], it is proven positivity can be removed for a much softer scaling than the one in (21).

The one-component problem, namely the derivation of the Gross-Pitaevskii equation

$$\mathrm{i}\partial_t u_t \;=\; -\Delta u_t + 8\pi a |u_t|^2 u_t,$$

has been an important open problem in mathematical physics in recent years. It was first solved by Erdős, Schlein and Yau in 2006 (see [4] and [5]); their proof was based on the BBGKY formalism and did not provide a convergence rate. Later results by Benedikter et al. [2] and by Pickl [21] relied on different techniques and allowed to get a quantitative control of the convergence.

3 Proof of Theorem 1

The strategy to get (15) is to establish an estimate of type

$$\partial_t \alpha^{(1,1)}_{N_1,N_2}(t) \leqslant f(t)\left(\alpha^{(1,1)}_{N_1,N_2}(t) + \frac{1}{N_1+N_2}\right), \tag{27}$$

and then to apply Grönwall lemma to get the result. The function f will depend on the population ratios c_1, c_2 and on certain norms of the potentials V_1, V_2, V_{12} and of the solutions u_t, v_t. For brevity, we will use from now on the shorthand notation $\alpha^{(1,1)} := \alpha^{(1,1)}_{N_1,N_2}(t)$.

One can show that our hypothesis certainly assure $\alpha^{(1,1)}$ to be differentiable in time; its derivative can be shown to split into three pieces, each one of them containing only one potential, according to

$$\dot{\alpha}^{(1,1)} \;=\; \mathrm{i}\,(C_{V_1} + C_{V_2} + C_{V_{12}}), \tag{28}$$

with

$$C_{V_1} := \Big\langle \Psi, \Big[\Big(\frac{1}{N_1}\sum_{i<j}^{N_1} V_1(x_i - x_j) - \sum_{i=1}^{N_1}(V_1^u)_i\Big)^A, \sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2}\frac{\mathbb{1} - p_k^A p_\ell^B}{N_1 N_2}\Big]\Psi\Big\rangle, \tag{29}$$

$$C_{V_2} := \Big\langle \Psi, \Big[\Big(\frac{1}{N_2}\sum_{r<s}^{N_2} V_2(y_r - y_s) - \sum_{r=1}^{N_2}(V_2^v)_r\Big)^B, \sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2}\frac{\mathbb{1} - p_k^A p_\ell^B}{N_1 N_2}\Big]\Psi\Big\rangle, \tag{30}$$

$$C_{V_{12}} = \Big\langle \Psi, \Big[\frac{1}{N_1+N_2} \sum_{i=1}^{N_1} \sum_{r=1}^{N_2} V_{12}(x_i - y_r) - c_2 \sum_{i=1}^{N_1} (V_{12}^{v})_i^A - c_1 \sum_{r=1}^{N_2} (V_{12}^{u})_r^B , \sum_{k=1}^{N_1} \sum_{\ell=1}^{N_2} \frac{\mathbb{1} - p_k^A p_\ell^B}{N_1 N_2} \Big] \Psi \Big\rangle . \tag{31}$$

Here and in what follows, the superscript A (respectively B) indicates that p_1^A acts on the first variable of the sector A, namely x_1 (respectively y_1). Each of these three summands will be estimated in terms of $\alpha^{(1,1)}$ and of $(N_1+N_2)^{-1}$ so as to obtain (27). The terms C_{V_1} and C_{V_2} contain only infra-species interactions, and, for this reason, their estimate is less involved; the detailed proof can be found in [12] (see also [9] for the single-component case).

To estimate $C_{V_{12}}$ one can exploit the bosonic symmetry of Ψ and the definition of c_j to obtain the bound

$$|C_{V_{12}}| \leqslant \frac{N_1 N_2}{N_1+N_2} \Big| \Big\langle \Psi, \Big[(V_{12})_{11} - (V_{12}^{v})_1^A - (V_{12}^{u})_1^B , \sum_{k=1}^{N_1} \sum_{\ell=1}^{N_2} \frac{p_k^A p_\ell^B}{N_1 N_2} \Big] \Psi \Big\rangle \Big| . \tag{32}$$

At this point, one is free to insert, on both sides of the commutator, the identity

$$\mathbb{1} = (p_1^A + q_1^A)(p_1^B + q_1^B), \tag{33}$$

with p and q as in (17), (18). The insertion clearly produces 16 terms, that we can split into two groups with a self-explanatory notation

$$\begin{aligned} \Lambda := \; & (pp,pp) + [(pq,pq) + (qp,qp)] + (qq,qq) \\ & + [(pq,qp) + \text{complex conjugate}] \end{aligned} \tag{34}$$

and

$$\begin{aligned} \Omega := \; & (pp,qp) + (qp,qq) + (pp,qq) + (pp,pq) + (pq,qq) \\ & + \text{ complex conjugate.} \end{aligned} \tag{35}$$

The terms (pp,pp), (qq,qq), $(pq,pq) + (qp,qp)$ in (34) vanish identically, which can be easily checked using the fact that $p_1^A q_1^A = 0$; all the others could, in principle, provide some contribution to (27). While we refer the reader to Sect. 5 in [12] for the detailed computation, we try to sketch here how each term can be handled.

Since we need to reconstruct $\alpha^{(1,1)} = 1 - \langle \Psi, p_1^A p_1^B \Psi \rangle$ [as in (27)], we can make a clever use of every $q_1^A \Psi$ or $q_1^B \Psi$ in the non-vanishing terms: indeed, $\|q_1^A \Psi\|^2 \leqslant \alpha^{(1,1)}$. For this reason, when at least one q from (33) appears on each side of the commutator, one only has to control the operator norm of $p_1 V_{12}(x_1 - y_1)$ and this allows to obtain the bound

$$\begin{aligned} &\Big| [(pq, qp) + \text{c.c.}] + [(qp, qq) + (pq, qq) + \text{c.c}] \Big| \\ &\qquad \leqslant f(t) \left(\alpha^{(1,1)}_{N_1,N_2}(t) + \frac{1}{N_1 + N_2} \right). \end{aligned} \tag{36}$$

The term (pp, qq) has the correct number of q's too, but they appear on the same side, and this would not allow to extract $\|q_1^A \Psi\|^2$; however, one q can be brought to the other side at the expense of some $(N_1 + N_2)^{-1}$ smallness. This allows to obtain

$$\Big| (pp, qq) + \text{c.c.} \Big| \leqslant f(t) \left(\alpha^{(1,1)}_{N_1,N_2}(t) + \frac{1}{N_1 + N_2} \right). \tag{37}$$

The only remaining term, (pp, qp), is the most important: in this case, only one q is surely not enough to re-create $\alpha^{(1,1)}$ and thus, some cancellation is needed to close the Grönwall estimate (27). Indeed, the key fact is that

$$p_1^B V_{12}(x_1 - y_1) p_1^B = p_1^B \Big(V_{12} * |v|^2 \Big)(x_1) p_1^B.$$

This "dressing" of the true potential V_{12} allows one to get an exact cancellation with the mean-field potential and obtain

$$(pp, qp) + \text{c.c.} = 0. \tag{38}$$

Collecting (36)–(38), one finally gets (27).

4 Proof of Theorem 2

To describe how the proof proceeds, we need to revisit more in detail the so-called "counting" method developed by Pickl. In order to get more compact expressions, we drop the subscript N_1, N_2 in α, Ψ, $\mathscr{E}$; the reader should keep in mind that everything always depends on the two population numbers. Given p_1^A and q_1^A as in (17) and (18), we define a new family of projectors: for each $k \in N$, take

$$P_k^A := \Big(q_1^A \dots q_k^A p_{k+1}^A \dots p_N^A \Big)_{sym}, \tag{39}$$

with the convention that $P_k^A = 0$ if $k > \mathbb{N}$ or $k < 0$; we remark that the symbol 'sym' in (39) denotes the mere sum (without normalisation factor) of all possible permuted versions of the considered string of projections. A perfectly analogous definition of P_k^B of course holds for the sector B. By definition, the range of P_k^A is the component of the Hilbert space in which exactly k particles of type A are in a state orthogonal to u (recall that $p = |u\rangle\langle u|$), that is to say outside of the condensate. Thus, $\| P_k^A \Psi \|^2 = \langle \Psi_{N_1,N_2}, P_k \Psi_{N_1,N_2} \rangle$ is a measure of how large the component of Ψ_{N_1,N_2} is, with exactly k particles of type A outside the condensate.

Now, given a positive function $g : \mathbb{N} \to \mathbb{R}$, define the operator

$$\widehat{g}^A := \sum_{k=0}^{N_1} g(k) P_k^A, \tag{40}$$

and the functional

$$\alpha^{(1,0)}_{N_1,N_2,g} := \langle \Psi_{N_1,N_2}, \widehat{g}^A \Psi_{N_1,N_2} \rangle. \tag{41}$$

This amounts to assign some weight $g(k)$ to the component of a many-body state with exactly k particles of type A outside the condensate, and then summing over k. In the same way one defines

$$\alpha^{(0,1)}_{N_1,N_2,g} := \langle \Psi_{N_1,N_2}, \widehat{g}^B \Psi_{N_1,N_2} \rangle. \tag{42}$$

The interest in this construction of course depends on the choice of g; it turns out that for some g's, convergence to zero of both $\alpha^{(1,0)}_{N_1,N_2,g}$ and $\alpha^{(0,1)}_{N_1,N_2,g}$ is equivalent to convergence in trace norm (25). This is true, for example, for the special choice of the weight function $s(k) := k/N$, which yields to the single-component analogous of (14).

4.1 The Functional $\boldsymbol{\alpha^{(1,0)}_{m,<}}$

Unfortunately, the scaling in (21) is too singular to allow one to close a Grönwall argument for the weight $s(k)$. We try to explain here all the modifications needed in order to get the machinery working. It turns out that, if one tries to perform calculations with the weight s, one gets

$$\left|\partial_t \langle \Psi, \widehat{s}^A \Psi \rangle\right| \leqslant C\Big(\langle \Psi, \widehat{s}^A \Psi \rangle + \langle \Psi, \widehat{n}^A \Psi \rangle + o(1) + \left|\mathscr{E}(\Psi) - \mathscr{E}^{GP}(u, v)\right|\Big),$$

where $n(k) := (k/N)^{1/2}$. Since $n(k) \geqslant s(k)$, the summand $\langle \Psi, \widehat{n} \Psi \rangle$ cannot be bounded and the estimate cannot be closed. This would suggest, in principle, that a Grönwall estimate could be proven only by choosing as functional to control

$$\widetilde{\alpha}^{(1,0)} := \langle \Psi, \widehat{n}^A \Psi \rangle + \left|\mathscr{E}(\Psi) - \mathscr{E}^{GP}(u, v)\right|. \tag{43}$$

We observe that the convergence to zero of such $\widetilde{\alpha}$ would allow again to obtain the statement in trace norm (25), since (see Lemma 6.1 in [21], adaptable to the two-component case)

$$\lim_{\substack{N_1\to\infty\\N_2\to\infty}} \langle\, \Psi,\ \widehat{n}\,\Psi\,\rangle = 0 \quad\Leftrightarrow\quad \lim_{\substack{N_1\to\infty\\N_2\to\infty}} \gamma^{(1,1)}(t) =\ |u_t\otimes v_t\rangle\langle u_t\otimes v_t|.$$

The functional $\widetilde{\alpha}$ is however not efficient enough yet; the reason is that its first and second derivative, which crucially enter in computations (see again [21], Appendix A.2), are singular for $k = 0$. For this reason, one defines a new weight, with a less singular behavior for small k's. For some fixed $\xi > 0$, we define

$$m(k) := \begin{cases} \sqrt{k/N}, & \text{for } k \geqslant N^{1-2\xi} \\ \\ \frac{1}{2}\big(N^{-1+\xi}k + x^{-\xi}\big), & \text{else.} \end{cases} \tag{44}$$

With this weight, we define a new functional as

$$\alpha_{m,<}^{(1,0)} := \langle\, \Psi,\ \widehat{m}^{A}\ \Psi\,\rangle + \big|\mathscr{E}(\Psi) - \mathscr{E}^{GP}(u,v)\big|. \tag{45}$$

The vanishing of this indicator and of its corresponding $\alpha_{m,<}^{(0,1)}$ is again equivalent to convergence in trace norm since

$$n(k) \leqslant m(k) \leqslant \max\{n(k), N^{-\xi}\}.$$

It turns out that $\alpha_{m,<}^{(1,0)}$ and $\alpha_{m,<}^{(0,1)}$ allow to control convergence for the softer scaling

$$V_N = N^{-1+3\beta}V(N^{\beta}(x-y)), \tag{46}$$

with $0 < \beta < 1$, but *not* for the true Gross-Pitaevskii scaling, corresponding to the case $\beta = 1$. The reason is that, for $\beta = 1$, an important role is played by the short-scale correlation among particles.

4.2 Adding Correlations

In the derivation of Gross-Pitaevskii equation, correlations are customarily accounted for (see for example [2]) by means of the solution f_N to the zero-energy scattering equation

$$\Big(-\Delta_x + \frac{1}{2}V_N(x)\Big)f_N(x) = 0, \qquad \text{with } f(x) \to 1 \ \text{ for } |x| \to \infty, \tag{47}$$

where $V_N(x) = N^2 V(Nx)$. In the setting we are considering, it is however more efficient [21] to consider a slight modification of (47). Recalling that we defined a_k as the scattering length of V_k for $k \in \{1, 2, 12\}$, we can define, for given constants C_j, C_{12}, the new potentials

$$W_{j,\beta}(x) := \begin{cases} \dfrac{4\pi a_j}{N_j} N_j^{3\beta}, & \text{for } N_j^{-\beta} < x < C_j N_j^{-\beta} \\ \\ 0 & \text{else}, \end{cases} \tag{48}$$

with $j \in \{1, 2\}$, and

$$W_{12,\beta}(x) := \begin{cases} 4\pi a_{12}(N_1 + N_2)^{3\beta-1}, & (N_1 + N_2)^{-\beta} < x < C_{12}(N_1 + N_2)^{-\beta} \\ \\ 0 & \text{else}. \end{cases} \tag{49}$$

One can show that there exist C_j, C_{12} such that the scattering lengths of $N_j^2 V(N_j^{\beta} \cdot) - W_{j,\beta}(\cdot)$ and of $(N_1+N_2)^2 V((N_1+N_2)^{\beta} \cdot) - W_{12,\beta}(\cdot)$ are zero (see Lemma 5.1 in [21] or Lemma 5.5 in [8] for a more detailed proof). One can now define two functions $f_{j,\beta}$ and $g_{j,\beta}$, $j = 1, 2$, by means of a modified zero-energy scattering equation, namely

$$\Big(-\Delta_x + \frac{1}{2}\big(V_{j,N_j}(x) - W_{j,\beta}(x)\big)\Big) f_{j,\beta}(x) = 0, \qquad \text{with } f_{j,\beta}(x) \to 1 \ \text{ for } |x| \to \infty, \tag{50}$$

and

$$g_{j,\beta} := 1 - f_{j,\beta}, \tag{51}$$

with the analogous definition for $f_{12,\beta}$ and $g_{12,\beta}$. By insertion of the new potential, it turns that out the norms of $g_{j,\beta}$ have a better behavior in $(N_1 + N_2)$ than they would have without the additional potential.

Now, by construction, the key properties of $W_{j,\beta}$ are

$$\|W_{j,\beta}\|_1 \sim O(N_1 + N_2)^{-1}, \quad \text{and} \quad \|W_{j,\beta}\|_\infty \sim O(N_1 + N_2)^{-1+3\beta},$$

and the same holds for $W_{12,\beta}$. For this reason, replacing $V_{j_N,j}$ (respectively V_{12,N_1+N_2}) in the proof with $W_{j,\beta}$ (respectively $W_{12,\beta}$) one would deal with a potential with a much less peaked scaling; of course the price to pay is the appearance of their difference, but this can be dealt with by adding a further term to the functional one aims to control.

Definition 1 ($\alpha_m^{(1,0)}$ **and** $\alpha_m^{(0,1)}$) We define *the* indicators of convergence for the Hamiltonian (21) as

$$\begin{aligned}\alpha_m^{(1,0)} := \alpha_{m,<}^{(1,0)} &- N_1(N_1-1)\mathrm{Re}\langle \Psi,\ g_{1,\beta}(x_1-x_2)\ R^A_{(12)}\psi \rangle \\ &- N_1N_2\mathrm{Re}\langle \Psi,\ g_{12,\beta}(x_1-y_1)\ R^A_{(12)}\psi \rangle\end{aligned} \tag{52}$$

and

$$\begin{aligned}\alpha_m^{(0,1)} := \alpha_{m,<}^{(0,1)} &- N_2(N_2-1)\mathrm{Re}\langle \Psi,\ g_{2,\beta}(y_1-y_2)\ R^B_{(12)}\psi \rangle \\ &- N_1N_2\mathrm{Re}\langle \Psi,\ g_{12,\beta}(x_1-y_1)\ R^B_{(12)}\psi \rangle,\end{aligned} \tag{53}$$

where $R_{(12)} := p_1p_2(\widehat{m}-\widehat{m}_2) + (p_1q_2+q_1p_2)(\widehat{m}-\widehat{m}_1)$, having used the shorthand notation $\widehat{m}_j := \sum_{k=0}^{N} m(k)P_{k+j}$.

Remark 6 The terms $\widehat{m}-\widehat{m}_1$ and $\widehat{m}-\widehat{m}_2$ are bounded in operator norm by $\sup_k |m'(k)|$. This is the reason why we had to define $m(k)$ by cutting $(k/N)^{1/2}$ for small k's.

Remark 7 The terms subtracted from $\alpha_{m,<}^{(1,0)}$ and $\alpha_{m,<}^{(0,1)}$ in Definition 1 are real but with no definite sign. However, one can easily prove a priori estimates for them; for example

$$N_1(N_1-1)\mathrm{Re}\langle \Psi,\ g_{1,\beta}(x_1-x_2)\ R^A_{(12)}\psi \rangle \le N^{-\eta}, \tag{54}$$

for some $\eta > 0$, and the same holds for the other four terms. This helps in closing the Grönwall estimate even though the considered functionals have no definite sign.

By repeating the computations in Appendix A.2 in [21] with minor changes, one can prove the estimate

$$\frac{d}{dt}\Big(\alpha_m^{(0,1)}(t) + \alpha_m^{(1,0)}(t)\Big) \leqslant f(t)\Big(\alpha_{m,<}^{(1,0)}(t) + \alpha_{m,<}^{(0,1)}(t) + (N_1+N_2)^{-\eta}\Big).$$

Now, by using the a priori estimate (54) and Grönwall Lemma, this is enough to get

$$\alpha_{m,<}^{(1,0)}(t) + \alpha_{m,<}^{(0,1)}(t) \leqslant e^{\int_0^t f(s)ds}\Big(\alpha_m^{(0,1)}(0) + \alpha_m^{(1,0)}(0) + N^{-\eta}\Big).$$

Since $\alpha_m^{(0,1)}(0) + \alpha_m^{(1,0)}(0)$ is converging to zero by Assumption (B3) and by Eq. (16) for $t = 0$, we get the thesis by using again Eq. (16) for $t > 0$.

5 Spinor Condensates and Other Multi-Component Models

As already remarked, the study of multi-component condensates is a very popular topic in theoretical and experimental physics; we would like to present in this section an account of some highly studied models, different from the mixture gas considered in this paper, that fall under the name of multi-component condensates.

In Sect. 2 we mentioned that a well-known example of multi-component condensate is a gas of spin bosons. Consider for example a system of atoms allowed to populate different hyperfine states; it is often assumed (and easily realizable with modern experimental techniques), that an external field is tuned in such a way that only two hyperfine levels are coupled and enter the effective Hamiltonian. When this is the case, then one can model the system by means of an auxiliary spin-1/2 bosonic theory. These systems are often referred to as *pseudo-spinor condensates*, since a proper spin-spin interaction is not present; nonetheless, the situation is already non trivial since one could even account for transitions between the two hyperfine levels: this can be realized for example by a (possibly time-dependent) external magnetic field. In this setting, the effective equations for the spin-1/2 case are (see for example [22, Sect. 21.3])

$$\begin{aligned} i\partial_t u_t &= -\Delta u_t + 8\pi a(|u_t|^2 + |v_t|^2)u_t + B(t)v_t \\ i\partial_t v_t &= -\Delta v_t + 8\pi a(|u_t|^2 + |v_t|^2)v_t + B(t)u_t, \end{aligned} \tag{55}$$

where a is the scattering length of the interaction and $B(t)$ is the magnetic field; the linear coupling provided by $B(t)$ is called *Rabi coupling*. We refer the reader to [13] for the derivation of (55) from the many-body dynamics of a pseudo-spinor condensate.

An even more interesting situation is the presence of spin-spin interaction. In the relevant case of a gas of alkali atoms, one should in principle take into account the presence of different values of hyperfine spin (e.g. $F = 1$ and $F = 2$); however, due to energetic arguments, a good low-energy approximation for the interaction can be obtained by completely neglecting the presence of one of the two hyperfine level, say $F = 2$. Under this approximation, it turns out that a general interaction Hamiltonian that preserves the hyperfine spin of the individual atoms and is rotationally invariant in the hyperfine spin space has the form

$$\delta(x_i - x_j)\big(c_0 + c_1 \mathbf{S_i} \cdot \mathbf{S_j}\big), \tag{56}$$

where $\mathbf{S_i}$ is the vector of spin-1 operators for the particle i. This not only provides population transfer, but it also correlates particles and for this reason the effect must be present on the non-linearity too. The factor $\delta(x_i - x_j)$ can be modeled by some Gross-Pitaevskii potential with scattering length c_1, and thus we can write the total spin-spin interaction term for a *spinor condensate* (neglecting the irrelevant c_0) as

$$N^2 \sum_{i<j} V(N(x_i - x_j))\mathbf{S_i} \cdot \mathbf{S_j}. \tag{57}$$

For the spin-1 case, this produces the equations [7, 17]

$$\begin{aligned} i\partial_t u_t &= -\Delta u_t + 8\pi a\Big(|v_t|^2 u_t + \overline{w}_t v_t^2 + |u_t|^2 u_t - |w_t|^2 u_t\Big) \\ i\partial_t v_t &= -\Delta v_t + 8\pi a\Big(|u_t|^2 v_t + 2\overline{v}_t w_t u_t + |w_t|^2 v_t\Big) \\ i\partial_t w_t &= -\Delta w_t + 8\pi a\Big(|v_t|^2 w_t + \overline{u}_t v_t^2 - |u_t|^2 w_t + |w_t|^2 w_t\Big), \end{aligned} \tag{58}$$

where again a is the scattering length of V. The rigorous derivation of the system (58) from many-body quantum dynamics is undoubtedly one of the next frontiers in the mathematics of the Bose gas.

Acknowledgements Partially supported by the 2014–2017 MIUR-FIR grant "*Cond-Math: Condensed Matter and Mathematical Physics*", code RBFR13WAET and by Gruppo Nazionale per la Fisica Matematica (GNFM-INdAM).

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Remarks on the Derivation of Gross-Pitaevskii Equation with Magnetic Laplacian

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Abstract The effective dynamics for a Bose-Einstein condensate in the regime of high dilution and subject to an external magnetic field is governed by a magnetic Gross-Pitaevskii equation. We elucidate the steps needed to adapt to the magnetic case the proof of the derivation of the Gross-Pitaevskii equation within the "projection counting" scheme.

Keywords Bose-Einstein condensate • Effective evolution equations • Gross-Pitaevskii scaling • Magnetic Gross-Pitaevskii equation • Magnetic Laplacian • Magnetic Sobolev space • Magnetic vector potential • Many-body quantum dynamics • Non-linear cubic Schrödinger equation • Reduced density matrix

1 Introduction and Result

The purpose of this note is to provide explicitly the non trivial adaptations of the known result [9] which are needed to prove the derivation of the so-called time-dependent magnetic Gross-Pitaevskii equation from the many-body Schrödinger dynamics of a dilute gas of identical bosons subject to an external magnetic field. The presentation is therefore somewhat technical; nonetheless, since, to our knowledge, no explicit details were so far available in the literature, we propose it as a reference for the increasingly interesting topic of the effective many-body quantum dynamics with magnetic field.

The rigorous derivation of the Gross-Pitaevskii equation has been over the last two decades a central topic in the mathematics of the Bose gas; in its essence, it is a problem of persistence of condensation, or propagation of chaos, in the following sense. Suppose that the initial datum of a three dimensional Bose gas displays condensation onto a one-body state $u_0 \in L^2(\mathbb{R}^3)$, namely

$$\lim_{N\to\infty} \gamma_{N,0}^{(1)} = |u_0\rangle\langle u_0|,$$

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A. Michelangeli, G. Dell'Antonio (eds.), *Advances in Quantum Mechanics*,
Springer INdAM Series 18, DOI 10.1007/978-3-319-58904-6_15

where $\gamma_{N,0}^{(1)}$ is the one-particle reduced density matrix associated to the initial datum $\psi_{N,0}$. Then condensation persists up to some time T if

$$\lim_{N\to\infty} \gamma_{N,t}^{(1)} = |u_t\rangle\langle u_t|, \quad \forall t \in [0,T],$$

for a condensate wave-function $u \equiv u_t(x)$ solution to the Gross-Pitaevskii equation

$$\mathrm{i}\partial_t u = -\Delta u + 8\pi a|u|^2 u$$

with initial datum u_0. Here a is the scattering length of the pair interaction among the particles of the many-body system.

The first complete proof of a result of this type is due to Erdős, Schlein, and Yau in 2006 (see [3, 4]); it was later reproduced with different methods by Pickl [9], by Benedikter, de Oliveira, and Schlein [1], and by Brennecke and Schlein [2]. All such derivations deal with a system of N interacting bosons in the Gross-Pitaevskii scaling limit with non-relativistic kinetic operator given by $-\Delta$; this corresponds to a many-body Hamiltonian of the form

$$H_N = \sum_{i=1}^{N}(-\Delta_i) + \sum_{i<j} N^2 V(N(x_i - x_j)).$$

Such methods can be adapted if the one-body Laplacian is modified by the insertion of an external (confining) potential. Analogously, it is of great relevance and interest to insert an external magnetic field which the charged particles are coupled with; mathematically this is modeled, with minimal coupling, by replacing the kinetic part in H_N with its magnetic counterpart

$$\sum_{i=1}^{N}(-\Delta_{\mathbf{A}})_i := \sum_{i=1}^{N}(-\mathrm{i}\nabla_i + \mathbf{A}(x_i))^2,$$

where $\mathbf{A} : \mathbb{R}^3 \to \mathbb{R}^3$ is a vector potential. This would in turn imply the effective dynamics to be ruled by the magnetic Gross-Pitaevskii equation

$$\mathrm{i}\partial_t u_t = -\Delta_{\mathbf{A}} u_t + 8\pi a|u_t|^2 u_t. \tag{1}$$

The fact that an external magnetic field can be accommodated into the many-body dynamics, and that the one-body marginal can be controlled analogously to what is done when the one-particle operator is simply the negative Laplacian, is to be expected and indeed is mentioned explicitly in [9, Remark 2.1]. However, such an adaptation is not as straightforward as the analogous insertion of an external trapping potential: the magnetic Laplacian is formally the sum of the ordinary Laplacian plus a derivative term that is linear in the magnetic potential and a further quadratic term in the magnetic potential itself; this more complicated structure requires an a priori not immediate adjustment of a number of crucial estimates and steps in the main proof. The related (simpler) problem of derivation of the magnetic Hartree equation from many-body quantum dynamics is dealt with in [7].

Before stating the result, let us define the magnetic Sobolev space $\mathrm{H}^k_{\mathbf{A}}$ as the set of $u \in L^2$ such that

$$\|u\|^2_{\mathrm{H}^k_{\mathbf{A}}} = \sum_{0\le j\le k} \|(\nabla - \mathrm{i}\mathbf{A})^j u\|_2^2 < +\infty.$$

We will consider the magnetic Hamiltonian

$$H_{N,\mathbf{A}} := -\sum_{i=1}^{N} \Delta_{i,\mathbf{A}} + \sum_{i<j} N^2 V(N(x_i - x_j)),$$

as the generator of the linear many-body Schrödinger dynamics. Moreover, we define the two **A**-dependent energy functionals

$$\mathcal{E}_N(\psi_N) := \frac{1}{N}\langle \psi_N, H_{N,\mathbf{A}}\psi_N\rangle \tag{2}$$

and

$$\mathcal{E}^{GP}(u) := \langle u, -\Delta_{\mathbf{A}} u\rangle + 4\pi a\langle u, |u|^2 u\rangle. \tag{3}$$

They represent the energies conserved along the flow of, respectively, the many-body Schrödinger equation and the magnetic Gross-Pitaevskii equation. We can now state the result as follows.

Theorem 1 *Let V be a positive, L^∞, spherically symmetric, and compactly supported function on $\mathbb{R}^3$, and let $\mathbf{A} \in W^{1,\infty}(\mathbb{R}^3, \mathbb{R}^3)$ be chosen such that $\nabla \cdot \mathbf{A} = 0$. Suppose that the sequence of initial many-body states $\{\psi_{N,0}\}_{N\in\mathbb{N}}$ is condensed in the sense of reduced densities, i.e.,*

$$\lim_{N\to\infty} \gamma^{(1)}_{N,0} = |u_0\rangle\langle u_0|$$

on a condensate wave-function $u_0 \in \mathrm{H}^2_{\mathbf{A}}$ (here $\gamma^{(1)}_{N,0}$ is the one-particle reduced density matrix of $\psi_{N,0}$). Suppose in addition that

$$\lim_{N\to\infty} \mathcal{E}_N(\psi_{N,0}) = \mathcal{E}^{GP}(u_0).$$

Then one has condensation for all $t > 0$, that is

$$\lim_{N\to\infty} \gamma^{(1)}_{N,t} = |u_t\rangle\langle u_t| \tag{4}$$

on a state u_t that solves the magnetic Gross-Pitaevskii equation (1) *with initial datum u_0. Here a is the scattering length of the interaction V.*

We remark that our hypotheses on $\mathbf{A}$ certainly ensures that $\|\cdot\|_{\mathrm{H}^k_{\mathbf{A}}}$ is equivalent to the standard Sobolev norm $\|\cdot\|_{\mathrm{H}^k}$ for $k \in \{0, 1, 2\}$; indeed, for any $f \in \mathrm{H}^2$, one has

$$\|\Delta_{\mathbf{A}} f\|_2 \lesssim \|\Delta f\|_2 + \|\mathbf{A}\|_\infty \|\nabla f\|_2 + \|\mathbf{A}\|_\infty^2 \|f\|_2 \lesssim \|f\|_{\mathrm{H}^2}$$

and, for any $f \in \mathrm{H}^2_{\mathbf{A}}$,

$$\|\Delta f\|_2 \lesssim \|\Delta_{\mathbf{A}} f\|_2 + \|\mathbf{A}\|_\infty \|\nabla f\|_2 + \|\mathbf{A}\|_\infty^2 \|f\|_2.$$

Since $\|\nabla f\|_2 \lesssim \epsilon \|\Delta f\|_2 + 1/\epsilon \|f\|_2$ for any $\epsilon > 0$, by choosing $\epsilon > 0$ small enough one gets $\|f\|_{\mathrm{H}^2} \lesssim \|f\|_{\mathrm{H}^2_{\mathbf{A}}}$. The cases $k = 0$ and $k = 1$ follow trivially.

We also stress that, again due to the hypotheses $\mathbf{A} \in W^{1,\infty}$ and $\nabla \cdot \mathbf{A} = 0$, the global existence of solution to the magnetic Gross-Pitaevskii equation (1) in the magnetic Sobolev spaces up to $k = 2$ is granted due to standard arguments. It would be of great interest to find a larger class of vector potentials such that a result similar to Theorem 1 holds: for example, a constant magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$ is not attainable by $\mathbf{A} \in W^{1,\infty}$.

An interesting future outlook is the derivation of the magnetic Gross-Pitaevskii equation for time-dependent magnetic potentials $\mathbf{A}(t)$. Since the treatment in [9] already deals with time-dependent external (electric) fields, it is expected that such result could be extended to cover a suitable class of $\mathbf{A}(t)$ having enough space and time regularity.

2 Proof of Theorem 1

Theorem 1 is proven with the same strategy as Theorem 2.1 in [9]. The crucial quantity one wants to control is

$$\alpha_{N,t} := \langle \psi_N, \widehat{m}\psi_N \rangle + |\mathcal{E}_N(\psi_N) - \mathcal{E}^{GP}(u)| - N(N-1)\mathrm{Re}\langle \psi_N, g_\beta(x_1 - x_2)\widehat{r}\psi_N \rangle. \tag{5}$$

For the definition of $\widehat{m}$ and $\widehat{r}$ in (5) see [9, Def. 6.1 and Def. 6.2]. The definition of g_β is recalled in eq. (10), since its role is slightly modified by the presence of $\mathbf{A}$. The core of the proof is to look for an estimate of the form

$$\partial_t \alpha_{N,t} \leq C(t)\Big(\langle \psi_N, \widehat{m}\psi_N \rangle + |\mathcal{E}_N(\psi_N) - \mathcal{E}^{GP}(u)| + N^{-\eta}\Big) \tag{6}$$

for some $\eta > 0$. By Grönwall Lemma, this is enough to get (4) (see [9, Sect. 6] for details). The factor $C(t)$, which varies from step to step during the proof, represents a function depending on the magnetic Sobolev norms $\|\psi_{N,t}\|_{\mathrm{H}^1_{\mathbf{A}}}$ and $\|u_t\|_{\mathrm{H}^2_{\mathbf{A}}}$; for this reason, it is in general exponentially growing in time, but not N-dependent.

Computing the time-derivative of $\alpha_{N,t}$ one gets

$$\partial_t \alpha_{N,t} \le \gamma_b + \gamma_c + \gamma_d + \gamma_e + \gamma_f + \gamma_l, \tag{7}$$

where the terms γ_j, $j \in \{b, c, d, e, f\}$ are defined in [5, Def. 6.6] and [9, Def. 6.3], while the new summand

$$\gamma_l := N^2 \big| \langle \psi_N,\ \nabla_{x_1} g_\beta(x_1 - x_2)\, \mathbf{A}(x_1) \widehat{r}\, \psi_N \rangle \big| \tag{8}$$

emerges in our case due to the presence of $\mathbf{A}$; let us remark that for us $\gamma_a = 0$ since we are not considering external traps.

In [9, Appendix A.2] it is shown in detail how γ_j, $j \in \{b, c, d, e, f\}$ (see [5, Sect. 6.4] for the estimate of γ_f) can be bounded in terms of $\langle \psi_N, \widehat{m}\psi_N \rangle$, $|\mathscr{E}_N(\psi_N) - \mathscr{E}^{GP}(u)|$ and $N^{-\eta}$, in order to obtain (6). We report in what follows the main adaptations needed in the magnetic case for the treatment presented in [9, Appendix A.2], plus the estimate of the additional term γ_l.

2.1 *Cancellation of the Kinetic Part*

A remarkable feature of the counting method we are considering here (introduced in [6, 8]) is that the single-particle terms in H_N (among them the kinetic part) get canceled exactly when computing $\partial_t \alpha_{N,t}$; in [9], this happens in Lemma 6.2 and it occurs in the case of $-\Delta_{\mathbf{A}}$ as well. More precisely, when computing $\partial_t \langle \psi_N, \widehat{m}\psi_N \rangle$, one has

$$\partial_t \langle \psi_N, \widehat{m}\psi_N \rangle = \mathrm{i} \Big\langle \psi_N, \Big[H_{N,\mathbf{A}} - \sum_{i=1}^{N} (-\Delta_{\mathbf{A},x_i} + 8\pi a |u|_i^2), \widehat{m} \Big] \psi_N \Big\rangle,$$

and one easily sees that the magnetic Laplacians get exactly canceled. This cancellation is the reason why, in the less involved mean-field case considered in [6], not much needs be done to deal with magnetic Laplacians. Apart from technical assumptions, all the proof proceeds in the same way since $-\Delta_{\mathbf{A}}$ does not play a role. In the Gross-Pitaevskii regime however, even though the cancellation takes place and the kinetic part does not have to be directly estimated, nonetheless $-\Delta_{\mathbf{A}}$ still plays a role along the proof through the emergence of the energy difference $|\mathscr{E}_N(\psi_N) - \mathscr{E}^{GP}(u)|$.

2.2 Cancellation of $V_N - W_\beta$

In analogy to the other known derivations of the Gross-Pitaevskii equation, one needs to include in the treatment a function displaying some short-scale structure that allows one to weaken the strong singularity of the interaction term $N^2V(N\cdot)$. This is done by means of the solution f_β to the zero-energy scattering problem relative to the modified potential $V_N - W_\beta$, where W_β is the less singular potential introduced in [9, Sect. 5] so as to make $V_N - W_\beta$ have zero scattering length. f_β is thus the solution to

$$\Big(-\Delta + \frac{1}{2}(V_N - W_\beta)\Big)f_\beta = 0, \tag{9}$$

with $f_\beta \to 1$ for $|x| \to \infty$. The function g_β that appears in (5) is defined as

$$g_\beta := 1 - f_\beta. \tag{10}$$

As explained in [9, Sect. 6.2], the function g_β plays a crucial role in the replacement of the strong potential V_N, which is of order N^2 at short distances, with the softer W_β, which is instead of order $N^{3\beta-1}$; this is of course at the expense of the appearance of their difference, but this can be shown to disappear exactly modulo terms that can be estimated. Performing all calculations for $\partial_t\alpha_{N,t}$ in the magnetic case, one gets as already mentioned the terms γ_b to γ_f as appearing in [9, Def. 6.3] and [5, Def. 6.6]; however, when computing $[H_N, g_\beta(x_1 - x_2)]$ as one can find after [9, Eq. 6.17], one gets

$$\begin{aligned}[H_N, g_\beta(x_1 - x_2)] =& [\Delta_{\mathbf{A},x_1} + \Delta_{\mathbf{A},x_2}, f_\beta(x_1 - x_2)] \\ =& (V_N - W_\beta)f_\beta(x_1 - x_2) - 2(\nabla_{x_1} g_\beta(x_1 - x_2))\nabla_{x_1} \\ & - 2(\nabla_{x_2} g_\beta(x_1 - x_2))\nabla_{x_2} - 2\mathrm{i}\mathbf{A}(x_1)(\nabla_{x_1} g_\beta(x_1 - x_2)) \\ & - 2\mathrm{i}\mathbf{A}(x_2)(\nabla_{x_2} g_\beta(x_1 - x_2)),\end{aligned} \tag{11}$$

having used $\nabla \cdot \mathbf{A} = 0$ and (9). The terms containing $(\nabla g_\beta)\nabla$ are present in [9] too, and they provide the term γ_c. The terms containing $\mathbf{A}$ were instead not present in the purely kinetic case, and they exactly correspond to γ_l.

2.3 Adapting the Estimates

To get the desired estimate (6) one has to treat separately γ_b, γ_c, γ_d, γ_e, γ_f, γ_l. The calculations proceed exactly as in [9, Appendix A.2], with some modifications we describe here.

2.3.1 Insertion of $h_{\beta_1,\beta}$

Lemma A.4 in [9] is used to prove the bound for γ_b and in its proof (to treat the term of type III for small β and of type I, II and III for arbitrary β) one replaces V_β with $U_{\beta_1,\beta} + \Delta h_{\beta_1,\beta}$; for example, one has (see [9, proof of Lemma A.4 (3), for β small])

$$N^2\big|\langle\psi_N, q_1p_2V_\beta(x_1-x_2)\widehat{m}q_1q_2\psi_N\rangle\big| \le N^2\big|\langle\psi_N, q_1p_2U_{0,\beta}(x_1-x_2)\widehat{m}q_1q_2\psi_N\rangle\big| + N^2\big|\langle\psi_N, q_1p_2(\Delta_1 h_{0,\beta}(x_1-x_2))\widehat{m}q_1q_2\psi_N\rangle\big|$$

The first summand can be bounded easily, since $U_{0,\beta}$ is less singular than V_β. To treat the second summand, the strategy is then to integrate by parts $\Delta h_{\beta_1,\beta}$ once or twice and then to manipulate the outcome in order to obtain the Sobolev norms of $\Psi_{N,t}$ or u_t. This procedure can be adapted to the magnetic case since one can use the trivial relation

$$\nabla = \nabla_{\mathbf{A}} + \mathrm{i}\mathbf{A},$$

which allows to get a magnetic gradient at the expense of a L^∞-bounded term. This allows to bound the second summand by

$$N^2\big|\langle\nabla_{1,\mathbf{A}}q_1p_2\psi_N, (\nabla_1 h_{0,\beta}(x_1-x_2))\widehat{m}q_1q_2\psi_N\rangle\big| \tag{12}$$

$$+ N^2\big|\langle\psi_N, q_1p_2(\nabla_1 h_{0,\beta}(x_1-x_2))\nabla_{1,\mathbf{A}}\widehat{m}q_1q_2\psi_N\rangle\big| \tag{13}$$

$$+ N^2\big|\langle\psi_N, q_1p_2\mathbf{A}(x_1)(\nabla_1 h_{0,\beta}(x_1-x_2))\widehat{m}q_1q_2\psi_N\rangle\big|. \tag{14}$$

At this point one can repeat the computations performed in [9] to bound the terms (A.14)–(A.17), the only difference being that $\nabla_{\mathbf{A}}$ will produce magnetic norms in the estimates of (12) and (13); (14) is even less singular, since it contains only one derivative, and it can again be bounded by repeating the bounds for [9, Eqs. A.14–A.17].

2.3.2 Magnetic Norms

The Sobolev norms $\|\psi_{N,t}\|_{\mathrm{H}^1}$ or $\|u_t\|_{\mathrm{H}^k}$ with $k = 1, 2$ emerge frequently along the proof, not only due to the integration by parts of $\Delta h_{\beta_1,\beta}$, but also typically by a Sobolev embedding argument (see e.g. [9, Eqs. A.37 and A.15]), or due to [9, Prop. A.3]. While in the non-magnetic case, such terms are bounded by some N-independent function of time, in the case of $\mathbf{A} \neq 0$ one needs to use the inequality $\|\cdot\|_{\mathrm{H}^k} \leqslant C\|\cdot\|_{\mathrm{H}^k_{\mathbf{A}}}$ granted by the equivalence of the two norms for $k = 1, 2$. Then, by general facts about magnetic Schrödinger equations, the two norms $\|\psi_{N,t}\|_{\mathrm{H}^1_{\mathbf{A}}}$ and $\|u_t\|_{\mathrm{H}^1_{\mathbf{A}}}$ are uniformly bounded in time. The magnetic Sobolev norm $\|\cdot\|_{\mathrm{H}^2_{\mathbf{A}}}$ is instead not a priori bounded, but the $W^{1,\infty}$-boundedness of $\mathbf{A}$ allows to get

$$\|u_t\|_{\mathrm{H}^2_{\mathbf{A}}} \leq De^{K|t|},$$

in the same way as for the non-magnetic case. The norm $\|u_t\|_\infty$ often appears as well, typically every time [9, Lemma 4.1 (5)] is used; $\|u_t\|_\infty$ can of course be bounded by $\|u_t\|_{\mathrm{H}^2}$ by standard embedding arguments, and hence by $C\,\|u_t\|_{\mathrm{H}^2_{\mathbf{A}}}$ again by equivalence of norms.

2.3.3 Lemma 5.2 of [9]

Lemma 5.2 in [9] allows one to bound a part of the kinetic energy by means of the functional $\alpha_{N,t}$ and $N^{-\eta}$; it plays a role in the estimate of the term of type III in Lemma A.4 of [9] and in the bound of γ_d [9, pp. 39–41]. It still holds in our case, with the substitution $\nabla \mapsto \nabla_{\mathbf{A}}$ and with the appropriate magnetic energy functionals defined in (2) and (3). In the proof (see [9, Appendix A.3]), one has exactly all the magnetic analogous of the terms [9, Eqs. A.53–A.60]. The term corresponding to [9, Eq. A.54] can be bounded by

$$\begin{aligned}
|\langle \nabla_{1,\mathbf{A}} q_1 \psi_N, \mathbb{I}_{\mathscr{A}_1} \nabla_{1,\mathbf{A}} p_1 \psi_N\rangle| &\leq |\langle \nabla_{1,\mathbf{A}} q_1 \psi_N, \nabla_{1,\mathbf{A}} p_1 \psi_N\rangle| \\
&\quad + |\langle \nabla_{1,\mathbf{A}} q_1 \psi_N, \mathbb{I}_{\overline{\mathscr{A}_1}} \nabla_{1,\mathbf{A}} p_1 \psi_N\rangle| \\
&\leq |\langle \widehat{n}^{-1/2} q_1 \psi_N, \Delta_{1,\mathbf{A}} \widehat{n}_1^{1/2} p_1 \psi_N\rangle| \\
&\quad + \|\mathbb{I}_{\overline{\mathscr{A}}_1}\|_{op} \|\nabla_{1,\mathbf{A}} q_1 \psi_N\| \|\nabla_{1,\mathbf{A}} p_1\|_{op} \\
&\leq C(t)\Big(\langle \psi_N, \widehat{n}\psi_N\rangle + N^{-\eta}\Big),
\end{aligned}$$

having used [9, Lemma 4.1 (3)] as well as the fact that $\widehat{n}^{-1/2}$ is well defined on $\operatorname{Ran} q_1$ for the second step and [9, Prop. A.1 (2)] for the third one. Here $\mathbb{I}_{\mathscr{A}_1}$ is the characteristic function of the set $\mathscr{A}_1$ defined in [9, Def. 5.2], while $C(t)$ is a function depending on the magnetic Sobolev norm $\|u_t\|_{\mathrm{H}^2_{\mathbf{A}}}$. With similar arguments one can bound the magnetic analogous of [9, Eq. A.59], i.e.,

$$\|\mathbb{I}_{\mathscr{A}_1} \nabla_{1,\mathbf{A}} p_1 \psi_N\|^2 - \|\nabla_{1,\mathbf{A}} u\|^2,$$

and this is enough to get the thesis of [9, Lemma 5.2] (the interaction terms are of course unmodified by the insertion of $\mathbf{A}$).

2.3.4 Bound on γ_l

We show here how the term γ_l defined in (8) can be estimated in order to get (6).

Lemma 1 *There exists* $\eta > 0$ *such that*

$$\gamma_l \leqslant C(t)\, N^{-\eta}$$

for a function $C(t)$ *depending on* $\|u_t\|_{H^2_{\mathbf{A}}}$ *but not on* N.

Proof We recall that

$$\widehat{r} := p_1 p_2 \widehat{m}^b + (p_1 q_2 + q_1 p_2)\widehat{m}^a,$$

where $\widehat{m}^b$ and $\widehat{m}^a$ are in [9, Def. 6.2]. By symmetry of g_β, we can integrate by parts in the x_2 variable; we get

$$\begin{aligned} |\gamma_l| \leqslant & N^2 \big| \langle \nabla_{x_2} \psi_N,\, g_\beta(x_1 - x_2)\, \mathbf{A}(x_1) \widehat{r}\, \psi_N \rangle \big| \\ & + N^2 \big| \langle \psi_N,\, g_\beta(x_1 - x_2)\, \mathbf{A}(x_1) \nabla_{x_2} \widehat{r}\, \psi_N \rangle \big|. \end{aligned} \tag{15}$$

We can use the definition of $\widehat{r}$ for the first term and get

$$N^2 \big| \langle \nabla_{x_2} \psi_N,\, g_{12}\, \mathbf{A}(x_1) \widehat{r}\, \psi_N \rangle \big| \leq N^2 \|\nabla_2 \psi_N\| \|\mathbf{A}\|_\infty \|g_{12} p_1\|_\infty (\|\widehat{m}^a\|_{op} + \|\widehat{m}^b\|_{op}),$$

having used the short-hand notation $g_{12} := g_\beta(x_1 - x_2)$. Now, by [9, Lemma 4.1], [9, Lemma 5.1] and [9, Eq. 6.11], one gets

$$N^2 \big| \langle \nabla_{x_2} \psi_N,\, g_{12}\, \mathbf{A}(x_1) \widehat{r}\, \psi_N \rangle \big| \leqslant C(t)\, N^{1+\xi} \|\psi_N\|_{H^1_{\mathbf{A}}} \|g_\beta\| \leqslant C(t) N^{-\beta/2+\xi},$$

for some $\xi > 0$ to be chosen suitably small. Here we used the uniform boundedness of the first magnetic Sobolev norm $\|\psi_N\|_{\mathrm{H}^1_{\mathbf{A}}}$ and the fact that $\|u_t\|_\infty$, produced by [9, Lemma 4.1], is bounded by $C\, \|u_t\|_{\mathrm{H}^2_{\mathbf{A}}}$.

As for the second term in (15), we can remark that two summands of $\widehat{r}$ contain p_1, and their sum is equal to $p_1 \widehat{r}$. For them, one can use Hölder inequality in the variable x_2 and then Sobolev inequality again in the variable x_2 to get

$$\begin{aligned} N^2 \big| \langle \psi_N,\, g_{12}\, \mathbf{A}(x_1) \nabla_{x_2} p_1 \widehat{r}\, \psi_N \rangle \big| \leqslant\ & N^2 \int d^3x_1\, d^3x_3 \ldots d^3x_N \|g_\beta(x_1 - \cdot)\|_{3/2} \\ & \times \|\psi_N(x_1, \cdot, x_3 \ldots x_N)\|_6 \|\mathbf{A}(x_1)(\nabla p_1 \widehat{r}\, \psi_N)(x_1, \cdot, x_3 \ldots x_N)\|_6 \\ & \leqslant N^2 \|g_\beta\|_{3/2} \|\mathbf{A}\|_\infty \int d^3x_1\, d^3x_3 \ldots d^3x_N \\ & \times \|\nabla \psi_N(x_1, \cdot, x_3 \ldots x_N)\| \|(\Delta p_1 \widehat{r}\, \psi_N)(x_1, \cdot, x_3 \ldots x_N)\| \\ & \leqslant C(t)\, N^2 \|\psi_N\|_{H^1_{\mathbf{A}}} \|g_\beta\|_{3/2} \|\Delta u\| (\|\widehat{m}^a\|_{op} + \|\widehat{m}^b\|_{op}), \end{aligned}$$

having used in the last step the definition of $\widehat{r}$, the fact that $\|\Delta p\|_{op} = \|\Delta u\|_2$ and [9, Cor. 4.1]. By interchanging the roles of x_1 and x_2, the same estimate can be proven if $q_1\widehat{r}$ replaces $p_1\widehat{r}$. One can now use $\|\Delta u\| \leqslant C\|u\|_{H^2_{\mathbf{A}}}$, [9, Lemma 5.1] (plus a standard interpolation argument to obtain $\|g_\beta\|_{3/2} \le \|g_\beta\|_2^{2/3} \|g_\beta\|_1^{1/3} \le CN^{-1-\beta_1}$) and [9, Eq. 6.11] and get

$$N^2 \big| \langle \psi_N,\ g_{12}\,\mathbf{A}(x_1)\nabla_{x_2}\widehat{r}\,\psi_N \rangle \big| \leqslant C(t)\,N^{-\beta+\xi},$$

which is enough to get the thesis.

Acknowledgements Alessandro Olgiati is Partially supported by the 2014–2017 MIUR-FIR grant "*Cond-Math: Condensed Matter and Mathematical Physics*", code RBFR13WAET and by Gruppo Nazionale per la Fisica Matematica (GNFM-INdAM). The author also warmly thanks the GSSI, for the kind hospitality and financial support during a visit in L'Aquila.

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On the Inverse Spectral Problems for Quantum Graphs

M. Olivieri and D. Finco

Abstract We review some aspects of inverse spectral problems for quantum graphs. Under hypothesis of rational independence of lengths of edges it is possible, thanks to trace formulas, to reconstruct information on compact and non compact graphs from the knowledge, respectively, of the spectrum of Laplacian and of the scattering phase. In the case of Sturm-Liouville operators defined on compact graphs and in general for differential operators on compact star-graphs, unknown potentials can be recovered from the knowledge of the spectrum of operators obtained imposing different boundary conditions.

Keywords Inverse problems • Inverse scattering problems • Sturm-Liouville operators • Quantum graphs

MSC 2010 35R30, 81U40, 34B24

1 Introduction

Quantum graphs are metric graphs provided with a selfadjoint operator that describes the dynamics of waves on the graph. The most natural application of a quantum graph is in the study of nanoscopic networks and their quantum properties, and in the new important area of technological development in quantum wires. Quantum graphs are in general good models for wave dynamics in thin structures, for example in the case of photonic crystals, or in chemistry for the study of dynamics of π-electrons in naphthalene molecule (see [7]).

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A. Michelangeli, G. Dell'Antonio (eds.), *Advances in Quantum Mechanics*,
Springer INdAM Series 18, DOI 10.1007/978-3-319-58904-6_16

In the present work we deal with the spectral problems of quantum graphs. (Direct) spectral problem is usually referred to the problem of obtaining the spectrum of an operator from information about the graph; instead the inverse spectral problem is in general referred to acquiring information about the graph from the knowledge of the spectrum of a selfadjoint operator defined on the graph.

We review some inverse problems under different sets of hypotheses. In the first section we introduce fundamental definitions concerning selfadjoint operators and quantum systems on graphs. In the second and third ones we study inverse problems on compact graphs and we answer to the question of which information on the graph we can recover with or without the hypothesis of rational independence of lengths of edges. In the fourth section we consider non compact graphs and search for the relations between the scattering on graph, its spectrum and its topological structure. The final section is dedicated to recovering potentials of Sturm-Liouville operators defined on compact graphs from spectra of different problems that are obtained varying boundary conditions at vertices. We present the same problem for general differential operator on compact star-shaped graphs.

2 Fundamental Definitions

A *graph* is a couple of at most countable sets: $\Gamma = (\mathcal{V}, \mathcal{E})$, with $\mathcal{V} = \{v_i\}_{i=1}^{V}$ set of *vertices* and $\mathcal{E} = \{e_i\}_{i=1}^{E}$ set of *edges*.

Every edge is a binary relation between two vertices: if $e \in \mathcal{E}$, then $e = \{v, w\} = \{w, v\}$, $v, w \in \mathcal{V}$; we say that the vertices v, w are *incident* to e and indicate it with $v, w \sim e$ (loops and multiple edges are also admitted, for example: $e = \{v, v\}$ is a loop).

With *oriented* graph we mean a graph in which an orientation has been defined on every edge. We will call *bonds* the oriented edges and indicate the set of bonds with $\mathcal{B}$, so if $b \in \mathcal{B}$, then $b = (v, w) \in \mathcal{V} \times \mathcal{V}$. The inverse bond of b is simply defined as $\bar{b} = (w, v)$. By definition, $\mathcal{B}$ contains the bonds and their inverse bonds (so $|\mathcal{B}| = 2E$), instead if we consider a precise orientation for every edge, we can indicate the set of such bonds always with $\mathcal{E}$, without considering the edges with inverse orientation. From now on we are going to consider only oriented graphs.

If we put an orientation on a graph it is possible to turn the graph into a metric system defining a length function. A *metric graph* is a graph with a length assigned to every bond: $L_b \in (0, +\infty]$ for every $b \in \mathcal{B}$ and the property that $L_b = L_{\bar{b}}$. So it is possible to define the length of every edge without contradiction: $L_e := L_b = L_{\bar{b}}$, if $b = (v, w)$ and $e = \{v, w\}$.

A *compact* graph is a graph with a finite number of edges with finite length, otherwise we will call it *non compact*.

On an edge e of a metric graph we can define a coordinate $x_e \in [0, L_e]$ and the respective Lebesgue measure dx_e (the coordinate increases following the orientation).

In the case of a quantum system we need to identify a Hilbert space $\mathcal{H}$ as space of states. In our case, if not specified otherwise, we will always take the Hilbert space associated to one particle moving on the graph

$$\mathcal{H} = L^2(\Gamma) := \bigoplus_{e\in\mathcal{E}} L^2(e, dx_e)$$

that is, a square-integrable function on a metric graph can be thought as a collection of E L^2-functions defined on every edge:

$$\psi := (\psi_1(x_1), \psi_2(x_2), \dots, \psi_E(x_E)), \quad x_1 \in [0, L_1], x_2 \in [0, L_2], \dots, x_E \in [0, L_E]$$

and so an operator on a graph acts on the set of these functions.

A *quantum graph* is a triple $(\Gamma, H, \mathcal{D}(H))$ with Γ metric graph, H a selfadjoint operator and $\mathcal{D}(H) \subseteq \mathcal{H}$ its domain.

A concrete example is given by the *Laplacian* on a metric graph, defined as

$$H := -\frac{d^2}{dx^2} = \left(-\frac{d^2}{dx_e^2}\right)_{e\in\mathcal{E}}$$

that acts on every edge as a second derivative. The next theorem from [2] guarantees conditions on its domain for selfadjointness, under reasonable physical hypotheses on graph structure (that from now on we will always assume). Let us denote the degree of a vertex v by d_v that is the number of edges incident to v, that we assume finite for every vertex:

$$d_v := |\{e \in \mathcal{E} : e = \{v, w\}, w \in \mathcal{V}\}|.$$

Theorem 2.1 *Let Γ be a metric graph with every length of edge bounded from below by a length L_0 (i.e. $0 < L_0 \leq L_e$, for every $e \in \mathcal{E}$), and H the Laplacian with domain $\mathcal{D}(H) \subseteq \mathcal{H}$. The operator H is selfadjoint on $\mathcal{D}(H)$ if and only if $\mathcal{D}(H)$ is the set of ψ such that:*

(i) *$\psi \in \bigoplus_{e\in\mathcal{E}} H^2(e, dx_e)$, with $H^2(e, dx_e)$ Sobolev space on edge e:*

$$H^2(e, dx_e) := \{\phi_e \in L^2(e, dx_e) : \phi_e'' \in L^2(e, dx_e)\};$$

(ii) *(vertices condition) for every $v \in \mathcal{V}$ exist $A_v, B_v \in Mat(d_v)$ such that*

- *$rk(A_v|B_v) = d_v$, with $(A_v|B_v)$ matrix that has as columns the union of columns of A_v and B_v;*
- *$A_v B_v^*$ is selfadjoint;*
- *$A_v\psi(v) + B_v\psi'(v) = 0$, where $\psi(v)$ is the vector $(\psi_1(v), \dots, \psi_{d_v}(v))$ of the components of ψ on the edges incident to v valued in the coordinate corresponding to v on the edge;*

and it is assumed that $\|B_v^{-1}A_vQ_v\|$ is uniformly bounded (where Q_v denotes the orthogonal projection onto the range of B_v^*, and B_v^{-1} is the inverse matrix of B_v acting from the range of B_v^* to the range of B_v).

So with the previous conditions, $(\Gamma, H, \mathcal{D}(H))$ is a quantum graph.

We observe that the vertices conditions are implicitly determined also by assigning a *scattering matrix* σ^v at each vertex v, defined as follows:

$$\sigma^v(k) := -(A_v + ikB_v)^{-1}(A_v - ikB_v), \quad k \in \mathbb{C}. \tag{1}$$

See [2] for the physical meaning of the scattering matrices and their relation with transmission through the vertices of waves moving along the graph.

Let us consider a particular case of conditions at vertices that assure selfadjointness thanks to the Theorem 2.1. We take for every vertex v

$$A_v = \begin{pmatrix} 1 & -1 & 0 & \dots & 0 & 0 \\ 0 & 1 & -1 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & 1 & -1 \\ 0 & 0 & \dots & \dots & 0 & 0 \end{pmatrix}, \quad B_v = \begin{pmatrix} 0 & 0 & \dots & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \dots & 0 & 0 \\ 1 & 1 & \dots & \dots & 1 & 1 \end{pmatrix}$$

and so we obtain *Kirchhoff-Neumann* (K-N) conditions: for every vertex v, ψ has to satisfy

$$\begin{cases} \psi \ \text{continuous in } v \\ \sum_{e\sim v} \psi_e'(v) = 0. \end{cases} \tag{2}$$

where the derivatives are taken in the outgoing direction from the vertex v and the continuity condition is: $\psi_1(v) = \dots = \psi_{d_v}(v)$.

In this case the scattering matrices are k-independent (so energy independent, see [2]) and their elements have the explicit form [8]:

$$\sigma^v_{i,j} = \frac{2}{d_v} - \delta_{i,j}, \tag{3}$$

where $\delta_{i,j}$ is the Kronecker delta.

3 Compact Graphs: Inverse Problem with Rational Independence of Edges Lengths

In this section we deal with the inverse spectral problem for compact quantum graphs. From now on Γ will be a metric compact graph, $(H, \mathcal{D}(H))$ the Laplacian with K-N conditions (from now on called as K-N Laplacian).

Under these hypotheses a *trace formula* exists that gives a relation between the spectrum of the Laplacian and the topological structure of the graph.

First of all let us remark that from [2] (Theorem 3.1.1) we have that the K-N Laplacian on a compact quantum graph has a discrete spectrum composed by positive eigenvalues with finite multiplicity and accumulation at infinity. So we can express the spectrum in this way:

$$\sigma(H) = \{k_n^2\}_{n\in\mathbb{N}} \subseteq \mathbb{R}, \qquad 0 = k_0^2 < k_1^2 \leq k_2^2 \leq \dots$$

Now we can define a distribution, the *spectral density* u:

$$u(k) := 2\delta(k) + \sum_{n=1}^{\infty}(\delta(k-k_n) + \delta(k+k_n))$$

and its Fourier transform:

$$\sqrt{2\pi}\hat{u}(l) = 2 + \sum_{n=1}^{\infty}(e^{-ik_nl} + e^{ik_nl}).$$

The trace formula gives an alternative formula for the spectral density and its transform involving periodic orbits on the graph (see [9]).

Theorem 3.1 *Let Γ be a metric, compact, connected graph and $(H, \mathcal{D}(H))$ the K-N Laplacian. Then the following trace formulas establish the relation between the spectrum $\sigma(H) = \{k_n^2\}_{n\in\mathbb{N}}$ of H and the set of periodic orbits, the total length and the Euler characteristic of the graph:*

$$u(k) = \chi\delta(k) + \frac{L}{\pi} + \frac{1}{2\pi}\sum_{p\in\mathcal{P}}(\mathcal{A}_p e^{ikl_p} + \mathcal{A}_p^* e^{ikl_p}), \tag{4}$$

$$\sqrt{2\pi}\hat{u}(l) = \chi + 2L\delta(l) + \sum_{p\in\mathcal{P}}(\mathcal{A}_p\delta(l-l_p) + \mathcal{A}_p^*\delta(l+l_p)), \tag{5}$$

where

$$\mathcal{A}_p = l_{p'}\left(\prod_{\sigma_{ij}^v\in\mathcal{T}(p)}\sigma_{ij}^v\right), \quad \mathcal{A}_p^* = l_{p'}\left(\prod_{\sigma_{ij}^v\in\mathcal{T}(p)}\overline{\sigma_{ij}^v}\right),$$

- *$\chi := V - E$ is the Euler characteristic of the graph;*
- *L : sum of the lengths of the edges of Γ, called the total length;*
- *$\mathcal{P}$ set of periodic orbits on Γ. A periodic orbit is an equivalence class of oriented closed paths invariant under the action of a cyclic permutation of edges of the path;*
- *p' primitive orbit of p. If p has a length multiple of lengths of other orbits, p' is the orbit among these ones that has the minimal length;*
- *l_p length of the orbit p;*
- *$\mathcal{T}(p)$ set of all scattering matrices elements $\sigma_{i,j}^v$ associated to vertices v and edges i, j that belong to the periodic orbit p.*

Knowledge of the spectrum allows one to define the spectral density, and thanks to the trace formula we obtain that the support of (5) is the set of the lengths of all periodic orbits of the graph. In [9], if we assume hypothesis of rational independence of edges lengths and cleaning of graph (absence of vertices with degree 2), an algorithmic procedure to recover information about the graph is presented. The most important steps are the definitions of three sets $\mathcal{L}'' \subseteq \mathcal{L}' \subseteq \mathcal{L}$ where:

- $\mathcal{L} := \{l_p \ : \ p \in \mathcal{P}\}$ is the set of the lengths of periodic orbits that can be obtained by the support of (5);
- $\mathcal{L}' := \left\{ l \in \mathcal{L} \ : \ \sum_{p \in \mathcal{P} : l = l_p} \mathcal{A}_p \neq 0 \right\}$ gives connectivity of the graph because it contains the lengths of the edges and combination of lengths of couples of edges that are connected;
- $\mathcal{L}'' := \{l \in \mathcal{L}' : l \leq 2L\}$, that is a finite set, and so one can find a basis of lengths such that any element of $\mathcal{L}''$ can be obtained as semi-integer combination of the elements of the basis. The basis with the minimal lengths is the set of the lengths of the edges of the graph or their double (depending if an edge forms a loop or not respectively).

And so it is possible to recover the edges lengths $\{L_e\}_{e \in \mathcal{E}}$ and how they are connected, i.e. it is possible to reconstruct the graph.

Theorem 3.2 *Let Γ be a compact, connected, quantum graph with $(H, \mathcal{D}(H))$ K-N Laplacian. If we suppose that*

(i) Γ is clean (no vertices of degree 2),
(ii) the lengths of the edges are rational independent,

then from the spectrum $\sigma(H)$ it is possible to reconstruct uniquely the graph Γ (that is, the lengths of edges and how they are connected).

In [4] a counterexample is produced that shows the failure of reconstruction of graphs without the hypothesis of rational independence. Let us take Γ_1 in Fig. 1 and K-N Laplacian $(H, \mathcal{D}(H))$.

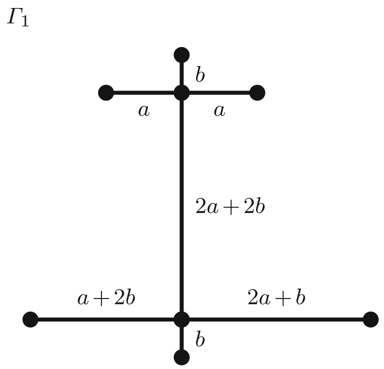
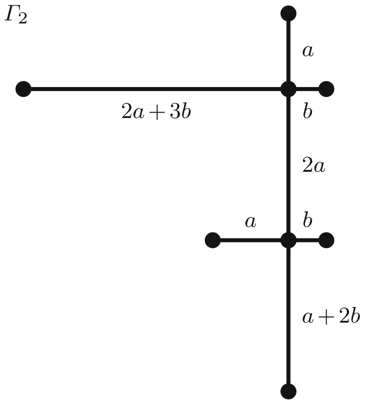


Fig. 1 Graph Γ_1

Fig. 2 Graph Γ_2



Its lengths are rational dependent. The spectrum of H is obtained solving the secular equation (see [4]), and consists of zeros of the function

$$f_1(k) = \tan(2(a+b)k) + \frac{2\tan(ak) + 2\tan(bk) + \tan((2a+b)k) + \tan((a+2b)k)}{1 - (2\tan(ak) + \tan(bk))(\tan(bk) + \tan((2a+b)k) + \tan((a+2b)k))}.$$

If we consider now $(H, \mathcal{D}(H))$ on graph Γ_2 in Fig. 2, always with rational dependence lengths, this time the spectrum of H consists of zeros of the function

$$f_2(k) = \tan(2ak) \cdot \frac{2\tan(ak) + 2\tan(bk) + \tan((a+2b)k) + \tan((2a+3b)k)}{1 - (\tan(ak) + \tan(bk) + \tan((a+2b)k)(\tan(ak) + \tan(bk) + \tan((2a+3b)k))}.$$

From [3] we have that zeros of f_1 and zeros of f_2 are the same, that is, Γ_1 and Γ_2 are isospectral graphs. So there is the failure of unique reconstruction of the graph from the spectrum of the Laplacian.

4 Compact Graphs: Inverse Problem in General

Now we do not assume the rational independence of edges lengths. Without this hypothesis only the Euler characteristic can be recovered (see [8]) and we have, thanks again to the trace formula, an explicit formula for χ.

Theorem 4.1 *Let Γ be a compact, connected, quantum graph with $(H, \mathcal{D}(H))$ the K-N Laplacian. Then from the spectrum $\sigma(H) = \{k_n^2\}_{n\in\mathbb{N}}$ it is possible to recover* *uniquely the Euler characteristic χ of the graph by the formula:*

$$\chi = 2 + 2 \lim_{t \to +\infty} \sum_{k_n \neq 0} \cos(k_n/t) \left(\frac{\sin(k_n/2t)}{k_n/2t} \right)^2 \tag{6}$$

$$= 2 - 2 \lim_{t \to +\infty} \sum_{k_n \neq 0} \frac{1 - 2\cos(k_n/t) + \cos(2k_n/t)}{(k_n/t)^2}. \tag{7}$$

It is possible to extend this result to bounded perturbation of the Laplacian (see [8]): let H_q be the operator

$$H_q = H + q, \quad \mathcal{D}(H_q) := \mathcal{D}(H).$$

where $q \in L^\infty(\Gamma)$ acts as a multiplication operator. H_q is selfadjoint in its domain and has a discrete spectrum: $\sigma(H_q) := \{(k'_n)^2\}_{n \in \mathbb{N}}$. Taking into account of the asymptotic formula $|k_n - k'_n| = O\left(\frac{1}{n}\right)$, where k_n^2 and $k_n'^2$ are the eigenvalues of H and H_q respectively, formula (6) still holds replacing k_n with k'_n.

Theorem 4.2 *Let Γ be a compact, connected, quantum graph with $(H_q, \mathcal{D}(H_q))$ the operator defined above. Then from the spectrum $\sigma(H_q) = \{(k'_n)^2\}_{n \in \mathbb{N}}$ it is possible to recover uniquely the Euler characteristic χ of the graph by the formula:*

$$\chi = 2 + 2 \lim_{t \to +\infty} \sum_{n=0}^{\infty} \cos(k'_n/t) \left(\frac{\sin(k'_n/2t)}{k'_n/2t} \right)^2 \tag{8}$$

5 Non Compact Graphs: Inverse Problem with Scattering

Now we are going to consider graphs with finite number of edges but also with infinite lengths. We deal with inverse problems for graphs that consist of a compact part and bonds of infinite length attached to some vertices and going to infinity. We call these bonds *leads*, their set $\mathcal{B}^{ext}$, and denote them with $(v, \infty) \in \mathcal{B}^{ext}$, with v vertex the lead is attached to (inverse bonds of leads are not admitted).

So the graph can be expressed in the form $\Gamma = (\mathcal{V}, \mathcal{B}),\ \mathcal{B} := \mathcal{B}^{int} \cup \mathcal{B}^{ext}$ where $\mathcal{B}^{int}$ are the bonds of the compact part.

Let us also make, for simplicity, the hypothesis of at most one lead attached to every vertex, so $|\mathcal{B}^{ext}| = N \leq V$. If we do not consider inverse bonds, we denote with $\mathcal{E} = \mathcal{E}^{int} \cup \mathcal{E}^{ext}$, $\mathcal{E}^{int}$ set of internal edges of compact part of the graph, and $\mathcal{E}^{ext}$ edges associated to leads (obviously $\mathcal{E}^{ext} = \mathcal{B}^{ext}$).

The eigenvalues problem for the Laplacian with general selfadjoint conditions at vertices

$$-\frac{d^2}{dx_b^2} \psi_b(x) = k^2 \psi_b(x), \quad b \in \mathcal{B}$$

on the bonds in the compact part of the graph has the solutions:

$$\psi_b(x) = \alpha_b e^{ikx_b} + \alpha_{\bar{b}} e^{ikL_b} e^{-ikx_b}, \quad \text{if } b \in \mathcal{B}^{int} \tag{9}$$

while on leads we are interested in solution of the form:

$$\psi_b(x) = C_b^{in} e^{-ikx_b} + C_b^{out} e^{ikx_b}, \quad \text{if } b \in \mathcal{B}^{ext}. \tag{10}$$

In [2] it is explained how are related the $2E$-vector of coefficients of outgoing waves from vertices $\alpha := \{\alpha_b\}_{b\in\mathcal{B}^{int}}$, the N-vectors of coefficients of waves that leave the graph on leads $C^{out} := \{C_b^{out}\}_{b\in\mathcal{B}^{ext}}$ and the ones that reach the graph on the leads $C^{in} := \{C_b^{in}\}_{b\in\mathcal{B}^{ext}}$:

$$\begin{pmatrix} C^{out} \\ \alpha \end{pmatrix} = \begin{pmatrix} R(k) & T_o(k) \\ T_i(k) & S(k) \end{pmatrix} \begin{pmatrix} C^{in} \\ \alpha \end{pmatrix} \tag{11}$$

where in the previous expression the matrix is $(2E+N)\times(2E+N)$ and

- $S(k)$ describes the evolution of waves inside the compact part of the graph;
- $R(k)$ describes the immediate reflection of waves from the graph (from leads into leads);
- $T_o(k)$ and $T_i(k)$ describe transmission from the compact part out and from the leads into the compact part correspondingly.

Solving Eq. (11) (see [2] for explicit calculation) we find that

$$C^{out} = \Sigma(k) C^{in}$$

where $\Sigma(k) := R(k) + T_o(k)(\mathbb{1} - S(k))^{-1} T_i(k)$ is the *scattering matrix*[1] ($\mathbb{1}$ is the identity matrix). The knowledge of this matrix gives the opportunity to obtain again a method of reconstruction of a metric graph. If we define the *scattering phase* Φ by

$$\Phi(k) := -i \log \det(\Sigma(k))$$

and the *resonance density* u by

$$u(k) := \frac{1}{2\pi} \frac{d\Phi(k)}{dk}$$

we have in this case a trace formula for the resonance density (see [6] and [5]).

[1]The scattering matrices defined in the previous chapter can be thought as a restriction of this one for compact graphs. In fact for compact graphs there are not the lead-transmission terms and in a proper base: $\Sigma = \mathrm{diag}(\sigma^1, \ldots, \sigma^V)$.

Theorem 5.1 *Let Γ be a non-compact, metric graph formed by a compact part with at most one lead attached to every vertex, $(H, \mathcal{D}(H))$ the K-N Laplacian and Σ the scattering matrix associated. The next formula holds for the resonance density:*

$$u(k) = \frac{\tilde{L}}{\pi} + \frac{1}{2\pi} \sum_{p \in \tilde{\mathcal{P}}} \left(\tilde{\mathcal{A}}_p e^{ikl_p} + \tilde{\mathcal{A}}_p^* e^{-ikl_p} \right)$$

where

$$\tilde{\mathcal{A}}_p = l_{p'} \left(\prod_{\sigma_{ij}^v \in \tilde{\mathcal{T}}(p)} \sigma_{ij}^v \right), \quad \tilde{\mathcal{A}}_p^* = l_{p'} \left(\prod_{\sigma_{ij}^v \in \tilde{\mathcal{T}}(p)} \overline{\sigma_{ij}^v} \right),$$

- *$\tilde{L}$ is the total length of the compact part of the graph: $\tilde{L} := \frac{1}{2} \sum_{b \in \mathcal{B}^{int}} L_b$;*
- *$\tilde{\mathcal{P}}$ is the set of periodic orbits in the compact part of the graph;*
- *p' primitive orbit of p;*
- *l_p the length of the orbit p;*
- *$\tilde{\mathcal{T}}(p)$ set of all scattering matrices σ^v associated to vertices that belong to the periodic orbit p in the compact part of the graph.*

From the knowledge of the scattering phase and under the same hypotheses of Kirchhoff-Neumann conditions, cleanliness and rational independence of lengths, it is possible to reconstruct uniquely the graph with the same algorithm (find the support of the Fourier transform of u, and from it the lengths of edges and connectivity).

Theorem 5.2 *Let Γ be a non-compact, connected, quantum graph with $(H, \mathcal{D}(H))$ K-N Laplacian, formed by a compact part with at most one lead attached to every vertex. If we suppose that*

(i) *Γ is clean,*
(ii) *the lengths of the edges are rational independent,*

then from the scattering matrix Σ it is possible to reconstruct uniquely the compact part of the graph Γ.

Also in this case it is possible to find some counterexamples. The impossibility of unique reconstruction holds also for more general operators than the Laplacian H: let Γ be a non-compact graph with a finite number of bonds and leads, and H_Q be the Schrödinger operator

$$H_Q := H + Q \tag{12}$$

$$H_Q \psi = \left\{ -\frac{d^2}{dx_e^2} \psi_e(x_e) + q_e(x_e) \psi_e(x_e) \right\}_{e \in \mathcal{E}}$$

where $Q = \{q_e\}_{e \in \mathcal{E}} \in L^1(\Gamma) := \bigoplus_{e \in \mathcal{E}} L^1(e)$, Q real-valued and on the leads b there is the further request

$$\int_b (1 + |x_b|)|q_b(x_b)|dx_b < +\infty.$$

We have seen that the knowledge of the scattering matrix allows to find the scattering phase and, with the hypothesis of rational independence, reconstruct the graph.

The results given below show that if one knows the scattering matrix associated to operator (12) without further hypotheses on lengths of edges, reconstruction is no more possible. Also information on the potential can not be obtained.

We remark the fact that if two scattering matrices Σ and Σ' are similar (see [10]) then the corresponding Schrödinger operators are unitarily equivalent. So the next results have to be intended up to unitary equivalence of operators and up to similarity for scattering matrices (for further details, see always [10]):

1. (Bargmann) the knowledge of the graph, the selfadjoint boundary conditions at the vertices and the scattering matrix Σ for the Schrödinger operator H_Q is generally not enough to determine the real-valued potential Q (for a proof see [1]);
2. the knowledge of the scattering matrix Σ for the K-N Laplacian is generally not enough to determine the topological structure of the graph uniquely;
3. the knowledge of the topological structure of the graph and of the scattering matrix Σ for the K-N Laplacian is generally not enough to determine the graph uniquely;
4. the knowledge of the graph, the real-valued potential Q and the scattering matrix Σ for the Schrödinger operator H_Q is generally not enough to determine the Schrödinger operator uniquely.

If not otherwise specified, the counterexamples are all shown in [10].

6 Inverse Problem for Sturm-Liouville Operators on Graphs: Recovering Potential

We now consider the problem of the reconstruction of the potential from the knowledge of the spectrum of the operator associated to various vertices conditions on compact graphs in the case of Sturm-Liouville operators, and then more in general for differential operators of a variable order.

Let $\Gamma = (\mathcal{V}, \mathcal{E})$ be a compact graph. We call

$$\mathcal{V}_0 := \{v \in \mathcal{V} : d_v = 1\}$$

the set of *external vertices*, i.e., the set of vertices of degree 1 ($|\mathcal{V}_0| = V_0$). The others are called *internal* and indicated with $\mathcal{V}_1$ ($|\mathcal{V}_1| = V_1$), so that

$$\mathcal{V} = \mathcal{V}_0 \cup \mathcal{V}_1, \quad V = V_0 + V_1.$$

Edges that are incident to external vertices are called *external edges* and indicated with $\mathcal{E}_0$ (the same for bonds).

A *cycle* is an ordered sequence of bonds $(b_1, b_2, \dots, b_n)$ such that they form a closed curve: $b_1 = b_n$. We indicate the set of edges whose bonds form a cycle with $\mathcal{E}_2$, instead the ones that do not form a cycle with $\mathcal{E}_1$. Obviously $\mathcal{E}_0 \subseteq \mathcal{E}_1$ because we are not considering inverse bonds.

We enumerate the edges as follows:

- $\mathcal{E}_0 := \{e_1, \dots, e_p\}$;
- $\mathcal{E}_1 := \{e_1, \dots, e_r\}$, $r \geq p, p = V_0$ (every external vertex is incident to only one external edge);
- $\mathcal{E}_2 := \{e_{r+1}, \dots, e_E\}$.

As in the previous cases, we assign lengths to edges and consider an orientation on the graph so that coordinates on the edges are well defined. Let us take a function $\psi = (\psi_e)_{e \in \mathcal{E}}$ with every $\psi_e \in AC(e)$, where $AC(e)$ is the set of absolutely continuous functions on e; we take $Q = (q_e)_{e \in \mathcal{E}} \in L^1(\Gamma)$ to play the role of potential.

We define the *Sturm-Liouville problem*:

$$-\frac{d^2}{dx_e^2}\psi_e(x) + q_e(x)\psi_e(x) = \lambda \psi_e(x), \quad e \in \mathcal{E} \tag{13}$$

with K-N conditions on every internal vertex, that here we rewrite for convenience: for every $v \in \mathcal{V}_1$

$$\begin{cases} \psi \ \text{ continuous in } v \\ \sum_{e \sim v} \psi_e'(v) = 0. \end{cases} \tag{14}$$

With the specification of conditions on external vertices, we can produce various associated problems:

- $L_0(\Gamma)$ *problem:* (13)–(14) problem with *Dirichlet* conditions on external vertices, that is: for every $v \in \mathcal{V}_0$

$$\psi_e(v) = 0, \quad \text{for every } \ e \sim v;$$

- $L_k(\Gamma)$ *problems,* $k = 1, \dots, p-1$: (13)–(14) problem with Dirichlet conditions on external vertices except for the vertex v_k, that has *Neumann* condition

$$\psi_e'(v_k) = 0, \quad \text{for every } e \sim v_k,$$
$$\psi_e(v) = 0, \quad \text{for every } v \in \mathcal{V}_0 - \{v_k\}, e \sim v;$$

- $L_\nu^\xi(\Gamma)$ *problems,* $\xi = r+1, \dots, E$; $\nu = 0, 1$: ξ identifies an edge e_ξ part of a cycle. Denoting with v_ξ the vertex with coordinate zero on e_ξ, the $L_\nu^\xi(\Gamma)$ problem is (13) problem with K-N conditions on every internal vertex but not in v_ξ. In v_ξ we have K-N condition involving every incident edge except e_ξ,[2] while along e_ξ, the problem with $\nu = 0$ corresponds to Dirichlet condition on v_ξ, while the problem with $\nu = 1$ corresponds to Neumann condition on v_ξ. In the external vertices there are Dirichlet conditions:

$$\begin{cases} \psi_{e_\xi}(v_\xi) = 0, & \text{if } \nu = 0; \\ \psi_{e_\xi}'(v_\xi) = 0, & \text{if } \nu = 1; \end{cases}$$
$$\psi_e(v) = 0, \quad \text{for every } v \in \mathcal{V}_0, e \sim v_k.$$

Every problem defined above gives a different spectrum of the operator $H_Q := -\frac{d^2}{dx^2} + Q$ as solution. Let us associate every spectral set to problems in this way:

Problems	**Eigenvalues sets**
$L_0(\Gamma)$	$\Lambda_0 := \{\lambda_{0n}\}_{n\geq 1}$
$L_k(\Gamma)$	$\Lambda_k := \{\lambda_{kn}\}_{n\geq 1}$
$L_\nu^\xi(\Gamma)$	$\Lambda_\nu^\xi := \{\lambda_{\nu n}^\xi\}_{n\geq 1}$

Knowledge of all this spectral sets allows one to recover an unknown potential of the H_Q operator, as stated in [11].

Theorem 6.1 *Let Γ be a metric, compact, graph, and $H_Q := -\frac{d^2}{dx^2} + Q$ a Schrödinger operator as previously defined. From the knowledge of*

- Λ_0 *;*
- Λ_k *for* $k = 1, \dots, p-1$*;*
- Λ_ν^ξ *for* $\xi = r+1, \dots, E$ *and* $\nu = 0, 1$

it is possible to recover uniquely the potential $Q = (q_e)_{e\in\mathcal{E}}$.

[2]So in the vertex v_ξ K-N conditions have to be rewritten as

$$\sum_{e_\xi \neq e \sim v_\xi} \psi_e'(v_\xi) = 0$$

.

Let us now deal with the case of general differential operators of variable order. In this case, if we admit also the presence of cycles, we have a result for star-shaped graphs.

Let $\Gamma = (\mathcal{V}, \mathcal{E})$ be a metric, compact star-shaped graph with a cycle, i.e. if $\mathcal{V} = \{v_0, \dots, v_{E-1}\}$ and $\mathcal{E} = \{e_0, \dots, e_{E-1}\}$ we suppose that $e_0 := (v_0, v_0)$ is a loop, and all the other edges are incident to v_0: $e_j := (v_j, v_0)$, with orientation in the direction entering in the vertex v_0 (so we can denote the edges simply with correspondent indices). Also in this case we take functions $\psi \in \bigoplus_{e\in\mathcal{E}} AC(e)$.

Fix numbers $2 = n_0 \leq n_1 \leq \dots \leq n_{E-1}$, and consider differential equations

$$\psi_j^{(n_j)}(x) + \sum_{\mu=0}^{n_j-2} q_{\mu j}(x)\psi_j^{(\mu)}(x) = \lambda\psi_j(x). \quad j = 0, \dots, E-1 \tag{15}$$

where $q_{\mu j} \in L^1(e)$ for every j, and so we have a potential $Q := \{q_{\mu j}\}$ with $j = 0, \dots, E-1$ and $\mu = 0, \dots, n_j - 2$.

Let us define conditions on the vertex v_0. First of all we introduce the linear forms

$$U_{j\nu}(\psi_j) := \sum_{\mu=0}^{\nu} \gamma_{j\nu\mu}\psi_j^{(\mu)}(L_j)$$

with $j = 1, \dots, E-1$; $\nu = 0, \dots, n_j - 1$ and $0 \neq \gamma_{j\nu\mu} \in \mathbb{C}$ are fixed complex numbers. Consider also the form

$$U_{0\nu}(\psi_0) := \psi_0^{(\nu)}(L_0), \quad \nu = 0, 1.$$

We define continuity conditions $C(\nu), C(0,\alpha)$ and Kirchhoff conditions $K(\nu)$ of order ν as follows:

- $C(\nu)$:

$$U_{E-1,\nu}(\psi_{E-1}) = U_{j\nu}(\psi_j), \quad j = 0, \dots, E-2;\ \nu < n_j - 1;$$

- $C(0,\alpha)$: $C(0)$ conditions and $\alpha\psi_0(0) = \psi_0(L_0)$;
- $K(\nu)$:

$$\sum_{j:\nu<n_j} \psi_j^{(\nu)}(L_j) = \delta_{1\nu}\psi_0'(0)$$

where δ_{jk} is the Kronecker delta and $\alpha \in \mathbb{C} - \{0\}$.

We define now, for fixed s, k, μ, with $s \in \{1, \dots, E-1\}, k \in \{1, \dots, n_s - 1\}$ and $\mu \in \{k, \dots, n_s\}$, the $L_{sk\mu}$ problem for the variable order differential operators. It can be defined as the problem (15) with

1. continuity conditions: $C(0, \alpha_s)$, $C(\nu)$, for $\nu = 1, \ldots, k-1$, and $K(\nu)$, for $\nu = k, \ldots, n_s - 1$ at the vertex v_0 (α_s being non-zero numbers at least two of which are different);
2. boundary conditions:

$$\psi_k^{(\nu-1)}(0) = 0, \quad \nu = 1, \ldots, k-1, \mu;$$

$$\psi_j^{(\nu-1)}(0) = 0, \quad \nu = 1, \ldots, n_j - k;\ j = 1, \ldots, E-1;\ j \neq s : n_j > k;$$

$$\psi_j(0) = 0, \quad j = 1, \ldots, E-1 : n_j \leq k$$

Solutions to these problems give discrete spectra $\Lambda_{sk\mu} := \{\lambda_{lsk\mu}\}_{l\geq 1}$, for $s = 1, \ldots, E-1; k = 1, \ldots, n_s - 1; \mu = k, \ldots, n_s$. Always from [11] we have a theorem of reconstruction of the potential Q.

Theorem 6.2 *Let Γ be a metric star-graph with a loop in the internal vertex. Consider Eq. (15) with associated $L_{sk\mu}$ problems, $s = 1, \ldots, E-1; k = 1, \ldots, n_s - 1; \mu = k, \ldots, n_s$ on the graph. Then from the knowledge of $\Lambda_{sk\mu}$, for every s, k, μ, it is possible to recover the unknown potential Q.*

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Double-Barrier Resonances and Time Decay of the Survival Probability: A Toy Model

Andrea Sacchetti

Abstract In this talk we consider the time evolution of a one-dimensional quantum system with a double barrier given by a couple of repulsive Dirac's deltas. In such a *pedagogical* model we give, by means of the theory of quantum resonances, the asymptotic behavior of $\langle \psi, e^{-itH}\phi \rangle$ for large times, where H is the double-barrier Hamiltonian operator and where ψ and ϕ are two test functions. In particular, when ψ is close to a resonant state then explicit expression of the dominant terms of the survival probability defined as $|\langle \psi, e^{-itH}\psi \rangle|^2$ is given.

Keywords Lambert special functions • Quantum resonances • Quantum survival probability • Singular barrier potential

1 Introduction

The phenomenon of exponential decay associated with quantum resonances is well known since the pioneering works on the Stark effect in an isolated hydrogen atom. Atomic hydrogen in an external electric field was first studied experimentally in 1913 by Stark [18] and Lo Surdo [11], and quantum mechanically in 1926 by Schrödinger [16]. The time independent Schrödinger equation for a hydrogen atom of nuclear charge Z, electron charge e, electron (reduced) mass m, in a uniform external electric field F directed along one axis (i.e. the z axis) has the form

$$H(F)\psi = \mathscr{E}\psi \, , \; H(F) := -\frac{\hbar^2}{2m}\Delta + \frac{eZ}{r} + Fez \, . \tag{1}$$

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A. Michelangeli, G. Dell'Antonio (eds.), *Advances in Quantum Mechanics*, Springer INdAM Series 18, DOI 10.1007/978-3-319-58904-6_17

When the external electric is absent, i.e. $F = 0$, then $H(0)$ has discrete negative eigenvalues given by (we set $\hbar = 1$, $2m = 1$ and $e = 1$)

$$\mathscr{E} = \mathscr{E}_{n,n_1,m} = -\frac{Z^2}{2n^2}$$

where $n = n_1 + n_2 + |m| + 1 = 1, 2, \dots$ is the *principal quantum number*, $|m| = 0, 1, 2, \dots, n-1$ and the quantum number n_1 is the number of nodes of the wave function.

In fact, when we switch on the electric field then the eigenvalues problem (1) has no eigenvalues at all as soon as $F \neq 0$. Thus, the quantum states experimentally observed in the Stark effect are not truly bound, but are instead *quantum resonances* associated with a *decay effect* of the *survival probability*. In fact, they are *s*hape resonances, which correspond to confinement of a particle by a barrier, through which tunneling occurs; although the strength of the electric field may be small, the perturbation interaction remains large somewhere far from the origin.

In order to explain the decay effect due to resonances let us consider, in a more general context, an Hamiltonian with a discrete eigenvalue $\mathscr{E}_0$ and an associated normalized eigenvector ψ_0. We suppose to weakly perturb such an Hamiltonian and that the new Hamiltonian H has purely absolutely continuous spectrum, that is the eigenvalue of the former Hamiltonian disappears into the continuous spectrum. Then we physically expect that, after a very short time, the *survival amplitude* has the following asymptotic behavior

$$\langle \psi_0, e^{-itH}\psi_0 \rangle \sim e^{-it\mathscr{E}} \tag{2}$$

where $\mathscr{E}$ is a quantum resonance close to the unperturbed eigenvalue $\mathscr{E}_0$, i.e. $\Re\mathscr{E} \sim \Re\mathscr{E}_0$ and $\Im\mathscr{E} < 0$ is such that $|\Im\mathscr{E}| \ll 1$. The *survival probability* is defined as the square of the absolute value of the survival amplitude (sometimes in the literature, with abuse of notation, both objects are named survival probability).

The validity of (2) has been proved when the perturbation term is given by a Stark potential. In such a case Herbst [10] proved that (2) holds true with an estimate of the error term. However, we should remark that Simon [17] pointed out that the exponentially decreasing behavior is dominant for large times only when the perturbed Hamiltonian H is not bounded from below. In fact, in the case of Hamiltonian H bounded from below we expect to observe a time decay for the survival amplitude of the form

$$\langle \psi_0, e^{-itH}\psi_0 \rangle = e^{-it\mathscr{E}} + b(t) \tag{3}$$

where the *remainder* term $b(t)$ is dominant for small and large times, and the exponential behavior is dominant for intermediate times. On the other hand, dispersive estimates for one-dimensional Schrödinger operators suggest that for large times the remainder term $b(t)$ is bounded by ct^{-r}, for some $c > 0$ and $r > 0$, as in the free model where $r = \frac{1}{2}$. However, this estimate is very raw because it does not take into account the resonances effects.

The analysis of the problem of the exponential decay rate *versus* the power decay rate in the time dependent survival amplitude defined by (3) is a research argument since the '50. In the seminal paper by Winter [20] it has been numerically conjectured that a transition effect between the two different kind of decays starts around some instant t. Recently a more rigorous analysis of the Winter's model, consisting of a one-dimensional model with one Dirac's delta potential at $x = R > 0$ and Dirichlet boundary condition at $x = 0$, has been done [7]. Such a transition effect has been also observed in ultra-cold sodium atoms trapped in an accelerating periodic optical potential [19]; more precisely, they show a transition from non-exponential decay for short times to exponential decay for intermediate time. Furthermore, Winter-like models, where a more general singular potential is considered, have been recently studied, see e.g. [4].

In this paper we consider a simple one-dimensional model with a symmetric double barrier potential with Hamiltonian

$$H_\alpha = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \alpha\delta(x+a) + \alpha\delta(x-a)$$

on the whole real axis [13, 14]. The two barriers are modeled by means of two symmetric repulsive Dirac's deltas at $x = \pm a$, for some $a > 0$, with strength $\alpha \in (0, +\infty]$. This model has been considered by [9], as a *pedagogical* model for the explicit study of quantum barrier resonances. However, H_α also has some physical interest as a model for ultra-thin double-barrier semiconductor heterostructures [12].

When $\alpha = +\infty$ the spectrum consists of a sequence of discrete eigenvalues $\mathcal{E}_{\infty,n}$, $n = 1, 2, 3, \ldots$, embedded in the continuum $[0, +\infty)$. When $\alpha < +\infty$ the spectrum of H_α is purely absolutely continuous and the eigenvalues obtained for H_∞ disappear into the continuum. More precisely, such eigenvalues becomes quantum resonances $\mathcal{E}_{\alpha,n}$ and the time decay of $\langle \psi, e^{-iHt}\phi \rangle$, where ψ and ϕ are two test functions, has the form (3) where

$$b(t) = c_\alpha t^{-3/2} + O(t^{-5/2}) \tag{4}$$

for large t and for some $c_\alpha > 0$ (see Theorem 1 below); in particular, in the case where the two test functions coincide with the unperturbed eigenvector then c_α may be explicitly computed (see Theorem 2 below) and it turns out that $c_\alpha \sim \alpha^{-2}$ in agreement with the fact that the asymptotic behavior (4) cannot uniformly hold true in a neighborhood of $\alpha = 0$.

In fact, we prove that a cancellation effect occurs and that the $t^{-1/2}$ factor coming from the free evolution propagator e^{-itH_0}, as usually occurs for the free one-dimensional Laplacian problem, is canceled by means of an opposite term coming from the two Dirac's deltas barrier. Hence, we can conclude that the effect of the double barrier is twice:

- the time-decay becomes faster, for t large for any $\alpha > 0$;
- for intermediate times the time-decay is slowed down because of the effect of the quantum resonant states.

Finally, we also find out the asymptotic value, for large α, of the instant t around which the transition between exponentially and power decay rate starts.

We should mention some papers where a weighted $t^{-3/2}$ dispersive estimate has been proved for the evolution operator under some assumptions on the potential. In particular, [8] (see also [15]) assumed that the potential is a L^1 function and that zero energy is not a resonance. We have to point out that the condition about the absence of zero energy resonance is crucial. In fact, in our model we see that the first resonance $\mathcal{E}_{\alpha,1}$ has limit zero when α goes to zero and the asymptotic behavior (4) does not hold true in such limit because c_α goes to infinity. We could overcome this problem by choosing the test vector ψ in a suitable subspace [3].

2 Description of the Model and Quantum Resonances

We consider the resonances problem for a one-dimensional Schrödinger equation with two symmetric potential barriers. In particular we model the two barriers by means of two Dirac's δ at $x = \pm a$, for some $a > 0$. The Schrödinger operator is formally defined on $L^2(\mathbb{R}, dx)$ as (let $\hbar = 1$ and $2m = 1$)

$$H_\alpha = -\frac{d^2}{dx^2} + \alpha\delta(x+a) + \alpha\delta(x-a)$$

where $\alpha \in (0, +\infty]$ denotes the strength of the Dirac's δ.

When $\alpha < +\infty$ it means that the wavefunction ψ should satisfies to the matching conditions

$$\psi(x+) = \psi(x-) \text{ and } \psi'(x+) = \psi'(x-) + \alpha\psi(x) \text{ at } x = \pm a\,, \tag{5}$$

and H_α has self-adjoint realization on the space of functions $H^2(\mathbb{R} \setminus \{\pm a\}) \cap H^1(\mathbb{R})$ satisfying the matching conditions (5). When $\alpha = +\infty$ it means that H_∞ has self-adjoint realization on a domain of functions satisfying the Dirichlet conditions $\psi(\pm a) = 0$. In this latter case then the eigenvalue problem $H_\infty\psi = \mathcal{E}_\infty\psi$ has simple eigenvalues $\mathcal{E}_{\infty,n} = k_n^2$ where $k_n = \frac{n\pi}{2a}$, $n = 1, 2, \ldots$, with associated (normalized) eigenvectors

$$\psi_n(x) = \begin{cases} 0 & \text{if } x < -a \\ \frac{1}{\sqrt{a}}\cos\left[k_n x - \frac{\pi}{4}(1 + (-1)^n)\right] & \text{if } -a < x < +a \\ 0 & \text{if } +a < x \end{cases} . \tag{6}$$

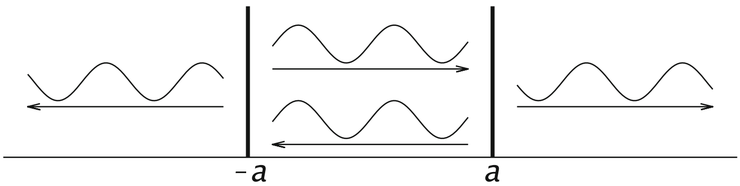

Fig. 1 Double-barrier model with two repulsive Dirac's δ at $x = \pm a$. Resonances are associated with the *outgoing* conditions $A = F = 0$ or, equivalently, to the poles of the kernel of the resolvent operator in the *unphysical complex half-plane* $\Im\mathscr{E} < 0$

The spectrum of H_∞ is then given by the continuum $[0, +\infty)$ with embedded eigenvalues $\mathscr{E}_{\infty,n}$.

In the case $\alpha \in (0, +\infty)$ then the eigenvalue problem

$$H_\alpha \psi = \mathscr{E}_\alpha \psi$$

has no real eigenvalues, but resonances; where resonances correspond to the complex values of $\mathscr{E}_\alpha$ such that the wavefunction

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{if } x < -a \\ Ce^{ikx} + De^{-ikx} & \text{if } -a < x < +a \\ Ee^{ikx} + Fe^{-ikx} & \text{if } +a < x \end{cases}, \; k = \sqrt{\mathscr{E}_\alpha}\,, \; \Im k \geq 0\,,$$

satisfying the matching condition (5), satisfies the *outgoing* conditions too (see Fig. 1)

$$A = 0 \text{ and } F = 0\,. \tag{7}$$

We should remark that the *outgoing condition* $A = F = 0$ implies that the wavefunction behaves like $e^{ik|x|}$ and thus it exponentially decays when the energy belongs to the *unphysical complex half-plane* $\Im\mathscr{E} < 0$.

The matching condition (5) and the resonance condition (7) imply that k satisfies to the following equation $M_{2,2} = 0$, where M is the transfer matrix $\begin{pmatrix} E \\ F \end{pmatrix} = M \begin{pmatrix} A \\ B \end{pmatrix}$. A straightforward calculation gives that equation $M_{2,2} = 0$ takes the form

$$\frac{1}{4k^2}\left[e^{4ika}\alpha^2 + 4k^2 + i4k\alpha - \alpha^2\right] = 0$$

that is

$$\left(e^{2ika}\alpha\right) \pm i\,(2k + i\alpha) = 0 \tag{8}$$

which has two families of complex-valued solutions

$$k_{1,m} = \frac{i}{2a}\left[W_m(-a\alpha e^{a\alpha}) - a\alpha\right] \text{ and } k_{2,m} = \frac{i}{2a}\left[W_m(a\alpha e^{a\alpha}) - a\alpha\right] \tag{9}$$

where $W_m(x)$ is the m-th branch, $m \in \mathbb{Z}$, of the Lambert special function. The Lambert function [2], denoted by $W(z)$ and introduced by Johann Heinrich Lambert (1728–1777), is defined to be the multivalued analytic function satisfying the equation $W(z)e^{W(z)} = z$, $z \in \mathbb{C}$.

It turns out that $\Im k_{j,m} < 0$ for any j and m, but $k_{2,0} = 0$, and thus equation $H_\alpha \psi = \mathscr{E}_\alpha \psi$ has no eigenvalues for any $\alpha > 0$. However, we have to remark that for $m < 0$ then $\Re k_{j,m} > 0$ and $\Im k_{j,m} < 0$ and then $\mathscr{E}_\alpha = \left(k_{j,m}\right)^2$ belongs to the *unphysical sheet* with $\Im \mathscr{E}_\alpha < 0$ for $m = -1, -2, -3, \ldots$. Therefore, we conclude that the spectral problem $H_\alpha \psi = \mathscr{E}_\alpha \psi$ has a family of resonances given by

$$\mathscr{E}_{\alpha,n} = \begin{cases} k^2_{1,-(n+1)/2} = \left[\frac{i}{2a}\left(W_{-\frac{n+1}{2}}(-a\alpha e^{a\alpha}) - a\alpha\right)\right]^2 & \text{if } n = 1, 3, 5, \ldots \\ k^2_{2,-n/2} = \left[\frac{i}{2a}\left(W_{-\frac{n}{2}}(a\alpha e^{a\alpha}) - a\alpha\right)\right]^2 & \text{if } n = 2, 4, 6, \ldots \end{cases} .$$

Let $a > 0$ be fixed, then it follows that for n fixed and α large enough the asymptotic behavior of the resonances follows from the asymptotic expansion of the Lambert function (see Eq. (4.18) by [2]) and it is given by (see [14] where the correct asymptotic expansion of the imaginary part of the resonance is reported)

$$\begin{aligned} \mathscr{E}_{\alpha,n} &= \left(\frac{n\pi}{2a}\right)^2 \left[1 - \frac{1}{a\alpha} + \frac{1}{a^2\alpha^2} - \frac{i}{a^2\alpha^2}\frac{n\pi}{2} + \mathscr{O}\left(\frac{1}{\alpha^3}\right)\right]^2 \\ &\sim \left(\frac{n\pi}{2a}\right)^2 - i\frac{n^3\pi^3}{4a^4\alpha^2} \end{aligned}$$

The explicit form of the resolvent of H_α, $\alpha \in (0, +\infty)$ is given by [1]

$$\left(\left[H_\alpha - k^2\right]^{-1}\phi\right)(x) = \int_{\mathbb{R}} K_\alpha(x, y; k)\phi(y)dy, \quad \phi \in L^2(\mathbb{R}),\ \Im k \geq 0\,,$$

where the integral kernel K_α is given by

$$K_\alpha(x, y; k) = K_0(x, y; k) + \sum_{j=1}^{4} K_j(x, y; k)$$

with $K_0(x, y; k) = \frac{i}{2k} e^{ik|x-y|}$ and $K_j(x, y; k) = L_j(x, y; k)/g(k)$ where $g(k) = 0$ is the resonance's equation,

$$g(k) := -2k\left((2k + i\alpha)^2 + \alpha^2 e^{i4ka}\right)\,,$$

and

$$L_1(x,y;k) = -\alpha(2k+i\alpha)\, e^{ik|x+a|} e^{ik|y+a|},\ L_4(x,y;k) = L_1(-x,-y;k)$$
$$L_2(x,y;k) = i\alpha^2\, e^{2ika}\ e^{ik|x+a|} e^{ik|y-a|},\ L_3(x,y;k) = L_2(-x,-y;k).$$

Resonances can be defined as the complex poles in the *unphysical sheet* $\Im \mathscr{E}_\alpha < 0$ of the kernel of the resolvent, too; that is the pole of the function $g(k)$ in agreement with (8).

3 Time Decay: Main Results

Let ϕ and ψ two well localized wave-functions, we are going to estimate the time decay of the term

$$\langle \psi, e^{-itH_\alpha}\phi\rangle \tag{10}$$

Theorem 1 *Let us assume that ϕ and ψ have compact support. Then we have that*

$$\langle \psi, e^{-itH_\alpha}\phi\rangle = c_\alpha t^{-3/2} + \sum_{n=1}^{\infty} \beta_n c_n e^{-i\mathscr{E}_{\alpha,n}t} + O(t^{-5/2}) \tag{11}$$

for some constants c_α and c_n and where

$$\beta_n = \begin{cases} 1 & \text{if } \left|\Im\sqrt{\mathscr{E}_{\alpha,n}}\right| < \left|\Re\sqrt{\mathscr{E}_{n,\alpha}}\right| \\ \frac{1}{2} & \text{if } \left|\Im\sqrt{\mathscr{E}_{\alpha,n}}\right| = \left|\Re\sqrt{\mathscr{E}_{\alpha,n}}\right| \\ 0 & \text{if } \left|\Im\sqrt{\mathscr{E}_{\alpha,n}}\right| > \left|\Re\sqrt{\mathscr{E}_{\alpha,n}}\right| \end{cases} . \tag{12}$$

We may remark that in the case $\alpha = 0$, that is when there are no barriers, then $\langle \psi, e^{-itH_0}\phi\rangle \sim t^{-1/2}$ and an apparent contradiction appears. The point is that the asymptotic expansion (11) is not uniform as α goes to zero. In fact, in an explicit model, see Theorem 2, it results that $c_\alpha \to \infty$ as $\alpha \to 0$. We can explain this apparent contradicion by remarking that the first resonance $\mathscr{E}_{\alpha,1} \to 0$ when $\alpha \to 0$ and that H_0 has a zero energy resonance.

Remark 1 Some authors [5, 6] discuss if and how the smoothness of the wave-functions ψ and ϕ plays a special role in the asymptotic behavior of the survival probability. Although this is a quite interesting question we don't treat it in such a paper.

We consider now, in particular, the asymptotic behavior of (10) when the test vectors ϕ and ψ coincide with one of the *localized* states, e.g. with $\psi_1(x) = \chi_{[-a,+a]}(x)\cos(k_1 x)$ defined by (6) for $n = 1$.

Theorem 2 *Let $\psi = \phi$ coinciding with the eigenvector ψ_1 of H_∞ associated with $\mathcal{E}_{\infty,1} = \left(\frac{\pi}{2a}\right)^2$, let $\ell(k)$ be the function defined as*

$$\ell(k) = 2\pi\sqrt{a}\frac{e^{2kai}+1}{\pi^2 - 4k^2a^2}\,, \tag{13}$$

and let $\mathcal{E}^2_{\alpha,1} = k_{1,-m}$ be the resonances defined by (9). Then

$$\langle \psi_1, e^{-itH_\alpha}\psi_1\rangle = c_\alpha t^{-3/2} + \sum_{m=1}^{\infty} \beta_m c_m e^{-i\mathcal{E}_{\alpha,1}t} + O(t^{-5/2}) \tag{14}$$

where β_m is defined by (12) and

$$c_\alpha = -\frac{2^{3/2}(1+i)a}{\pi^{5/2}\alpha^2}\,,\quad c_m = -\frac{\alpha\ell(k_{1,-m})^2}{1+\alpha a\left(1+\frac{2k_{1,-m}}{i\alpha}\right)}$$

This result agrees with the limit case when $\alpha = +\infty$. Indeed, we check that

$$\ell(k_{1,-m}) = \frac{4i\pi\sqrt{a}k_{1,-m}}{\alpha(\pi^2 - 4k^2_{1,-m}a^2)}$$

Hence

$$\ell(k_{1,-m}) \sim O(\alpha^{-1}) \text{ if } m \neq 1$$

as $\alpha \to +\infty$. For $m = 1$, from the asymptotic behavior of $k_{1,-1}$ it follows that

$$\pi^2 - 4k^2_{1,-1}a^2 \sim \pi^2 - 4a^2\left[\frac{\pi^2}{4a^2}\left(1 - \frac{2}{a\alpha}\right)\right] = \frac{2\pi^2}{a\alpha}$$

and then

$$\ell(k_{1,-1}) \sim i\sqrt{a}\,,\ \text{ as } \alpha \to +\infty\,.$$

Hence, as α goes to infinity it follows that the dominant term of $\langle \psi_1, e^{-itH_\alpha}\psi_1\rangle$ is given by

$$\langle \psi_1, e^{-itH_\alpha}\psi_1\rangle = e^{-i\left(\frac{\pi}{2a}\right)^2 t} + O(\alpha^{-1})$$

in agreement with the fact that $\langle \psi_1, e^{-iH_\infty t}\psi_1\rangle = e^{-i\mathcal{E}_{\alpha,1}t}$.

The proof of the Theorems is given by [13] and it is based on the explicit calculation of the evolution operator, obtained by the expression of the kernel of the resolvent operator, on the stationary phase theorem and the residue theorm.

4 Decay Transition

Let us compare, in the limit of large α and a fixed such that $a\alpha \gg 1$, the absolute values of the two dominant terms of $\langle \psi_1, e^{-itH_\alpha}\psi_1\rangle$ given by (14); that is the power term $\frac{d_1}{\alpha^2 t^{3/2}}$, where $d_1 = \left| \frac{2^{3/2}(1+i)a}{\pi^{5/2}} \right| = \frac{4a}{\pi^{5/2}}$, and the exponential term

$$\left| c_1 e^{-i\mathscr{E}_{\alpha,1}t} \right| = d_3 e^{\Im \mathscr{E}_{\alpha,1}t} \sim d_3 e^{-d_2 t/\alpha^2} ,$$

where

$$d_2 = \frac{\pi^3}{4a^4} \text{ and } d_3 = |c_1| = \left| \frac{\alpha \ell (k_{1,-1})^2}{1 + \alpha a \left(1 + \frac{2k_{1,-1}}{i\alpha}\right)} \right| \sim 1 .$$

In order to understand when the power behavior dominates and when the exponential behavior dominates we have to solve the inequality

$$\frac{d_1}{\alpha^2 t^{3/2}} < d_3 e^{-d_2 t/\alpha^2} .$$

A straightforward calculation gives that this inequality is satisfied for any $t \in [t_1, t_2]$, where $0 < t_1 < t_2$ are given by

$$t_1 = -\frac{3\alpha^2}{2d_2} W_0(z) \text{ and } t_2 = -\frac{3\alpha^2}{2d_2} W_{-1}(z) \tag{15}$$

where

$$z = -\frac{2}{3} \frac{d_2 d_1^{2/3}}{\alpha^{10/3} d_3^{2/3}} .$$

This interval is not empty provided that the argument z of the Lambert function is between $(-1/e, 0)$; which holds true for α large enough. Furthermore, we should remark that

$$t_1(\alpha) \sim \frac{d_1^{2/3}}{\alpha^{4/3} d_3^{2/3}} \ll 1 \text{ and } t_2(\alpha) \gg 1$$

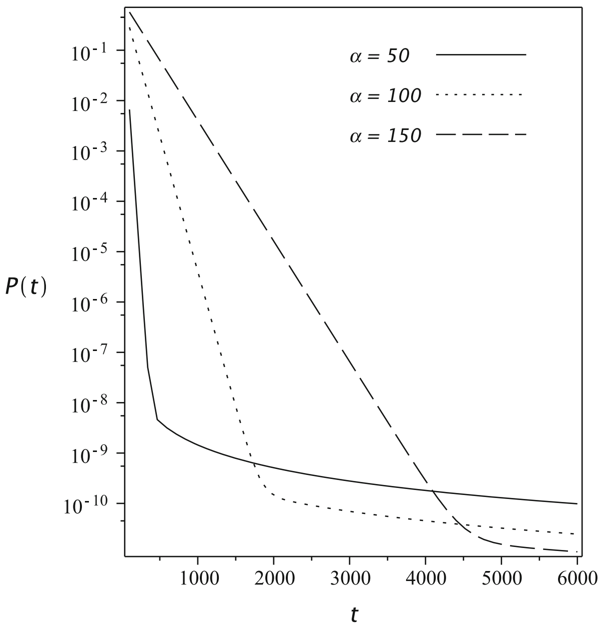

Fig. 2 Plot of the absolute value of the survival amplitude $P(t) = \left|\langle \psi_1, e^{-itH_\alpha}\psi_1\rangle\right|$ given by the dominant terms of (14) for large times $t \in [100, 6000]$ and for different values of α, here we fix $a = \frac{1}{2}$. Around $t = t_2(\alpha)$ a transition of the decay law starts; for $t < t_2(\alpha)$ the exponential decay dominates, while for $t > t_2(\alpha)$ the power law decay dominates

because $W_0(\zeta) \sim \zeta$ if $|\zeta| \ll 1$ and

$$W_{-1}(-\xi) \sim \ln(\xi) - \ln(-\ln(\xi))$$

if $0 < \xi \ll 1$.

Finally, we can resume these results in the following statement.

Proposition (decay transition) *Let $\alpha > 0$ be large enough, and let $t_2(\alpha)$ given by (15). Let $\langle \psi_1, e^{-itH_\alpha}\psi_1\rangle$ be the survival amplitude of the state ψ_1 given by (14) and consisting by a superposition of the exponential and power law decay terms. Then a transition from the exponential to the power law decay term starts around $t_2(\alpha)$. More precisely, for $t < t_2(\alpha)$ the exponential decay term dominates, while for $t > t_2(\alpha)$ the power law decay term dominates (see Fig. 2).*

Acknowledgements I'm very grateful to Sandro Teta for fruitful discussions. I thank very much Gian Michele Graf and Kenji Yajima for useful comments to my talk. This work is partially supported by Gruppo Nazionale per la Fisica Matematica (GNFM-INdAM).

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