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Editors

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Contents

Preface

This volume contains the proceedings of the conference *Spectral Theory and Mathematical Physics*, which took place at Pontificia Universidad Católica de Chile (PUC), Santiago, in November 2014. The main purpose of this conference was to bring together a number of established specialists in spectral theory and mathematical physics, as well as some young and beginning researchers in this field in order to connect people from different schools and generations, give them the opportunity to exchange ideas, and try to attract more young mathematicians to this fascinating area of research.

The conference Spectral Theory and Mathematical Physics and the preceding course on random Schrödinger operators given by Werner Kirsch and Ivan Veselić were organized within the framework of the International Spectral Network, financed in the Chilean side by Iniciativa Científica Milenio (ICM) of the Chilean Ministry of Economy. All the organizers belong to the Millennium Nucleus in Mathematical Physics RC120002. They gratefully acknowledge the financial support of ICM through the project Networking 2013, as well as support of the other conference sponsors: the Vice-Rectory of Research and the Faculty of Mathematics of PUC, the International Association of Mathematical Physics, and the Chilean Science Foundation FONDECYT. Special gratitude is due to the administrative staff of the Faculty of Mathematics of PUC for logistic help in organization of the conference.

We would like to thank the conference mini-course lecturers Serge Richard (Nagoya) and Fedor Sukochev (Sydney); our invited speakers: Jean-Marie Barbaroux (Toulon), Virginie Bonnaillie-Noël (Rennes), Vincent Bruneau (Bordeaux), Horia Cornean (Aalborg), Rafael del Rio (Mexico), Erdal Emsiz (Santiago), Claudio Fernández (Santiago), Dietrich Häfner (Grenoble), Werner Kirsch (Hagen), Hynek Kovařík (Brescia), David Krejčiřík (Prague), Alexander Nazarov (St. Petersburg), Rolando Rebolledo (Santiago), Thomas Sørensen (Munich), Matěj Tušek (Prague), and Ivan Veselić (Chemnitz); and the students who gave talks: Harold Bustos (Santiago), Fabien Clivaz (Zürich), Dhriti Dolai (Chennai), Tomás Lungenstrass (Santiago), Joseph Mehringer (Munich), Daniel Parra (Lyon), and Hanne van den Bosch (Santiago).

This volume contains survey articles as well as original results presented at the conference. Most of the articles are dedicated to some of the following topics:

- Ergodic Quantum Hamiltonians
- Magnetic Schrödinger Operators
- Quantum Field Theory
- Scattering Theory
- Semiclassical and Microlocal Analysis
- Spectral Shift Function and Quantum Resonances

As editors, we are grateful to the authors who contributed to this book, and to all the anonymous referees for their professional and time-consuming work. We would also like to thank Liliya Simeonova for handling manuscripts and referee reports and for technical assistance in the preparation of the volume.

The proceedings *Spectral Analysis of Quantum Hamiltonians* of the conference held in Santiago in 2010, were published in the Birkhäuser series *Operator Theory Advances and Applications* in 2012. The present publication is the second of what we hope to be a series of proceedings of regular conferences on spectral theory held in Santiago de Chile.

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Lower Bounds for Sojourn Time in a Simple Shape Resonance Model

J. Asch, O. Bourget, V.H. Cortés and C. Fernández

Abstract. We consider a simple model for shape resonance in the spirit of Gamov and prove that the sojourn time diverges as the square root of the height of the barrier. This result illustrates the power of Lavine's lower bound theory.

Mathematics Subject Classification (2010). 35P99, 81Q15.

Keywords. Quantum resonances, lifetime estimates.

1. Introduction

Shape resonances have been studied since the youth of quantum mechanics in order to explain radioactive decay, see, e.g., [4]. To be specific, consider the Schrödinger operator

$$H_a = -\frac{d^2}{dx^2} + V_a \,,$$

on the positive half-axis with Dirichlet boundary condition at zero and a potential bump V_a of height $a > 0$, compactly supported away from the origin and an energy $E < a$.

Gamov observed that an initial state φ of energy E, supported between the Dirichlet wall and the potential, decays in time with a rate proportional to $\sqrt{a-E}$ (see [4]). In the present contribution, we show that a lower bound proportional to $\sqrt{a-E}$ holds for the sojourn time of such states for a specific family of real-valued potentials $(V_a)_{a\geq 0}$ (see Theorem 2.1). We achieve this by using Lavine's lower bound theory, which is recalled in Section 2. The proof is developed in Section 3.

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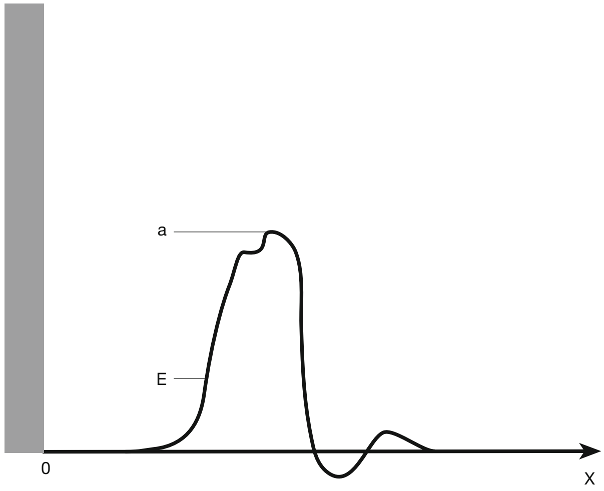

FIGURE 1. Potential bump of height a

2. Preliminaries and main result

2.1. The model

We recall the main features of the model introduced in [3]. We study specifically the family of Schrödinger operators $(H_a)_{a\geq 0}$ defined on $\mathcal{H} := L^2(0,\infty)$ with Dirichlet boundary conditions at 0 by

$$H_a = -\frac{d^2}{dx^2} + V_a = -\Delta + V_a, \tag{2.1}$$

where $V_a = aV$ and V is the function defined on $[0,\infty)$ by:

$$V(x) = \begin{cases} 0 & \text{if } x \in [0,\pi) \cup (\pi + b, \infty) \\ 1 & \text{if } \pi \leq x \leq \pi + b \end{cases} \tag{2.2}$$

with $b > 0$ fixed. The common domain of self-adjointness $\mathcal{D}_0$ of the family (H_a) is given by:

$$\mathcal{D}_0 = \left\{ \phi \in L^2(0,\infty); \phi, \phi_x \text{ a.c.}, \phi_{xx} \in L^2(0,\infty), \phi(0) = 0 \right\},$$

where a.c. means absolutely continuous.

For all $a \geq 0$ the spectrum of H_a is purely a.c. and is given by: $\sigma(H_a) = [0,\infty)$ (see [2]). In the limit when a tends to infinity, we introduce the self-adjoint operator H_∞ defined on the Hilbert space $\mathcal{H}_\infty := L^2_D(0,\pi) \oplus L^2_D(\pi + b, \infty)$ by $H_\infty = H_{\text{in}} \oplus H_{\text{out}}$ where H_{in} and H_{out} denote the Laplace operator $-\Delta$ defined respectively on the domains:

$$\mathcal{D}_{\text{in}} = \{\phi \in L^2(0,\pi); \phi, \phi_x \text{ a.c.}, \phi_{xx} \in L^2(0,\pi), \phi(0) = 0 = \phi(\pi)\},$$

$$\mathcal{D}_{\text{out}} = \{\phi \in L^2(\pi + b,\infty); \phi, \phi_x \text{ a.c.}, \phi_{xx} \in L^2(\pi + b,\infty), \phi(\pi + b) = 0\}.$$

The spectrum of H_{out} is purely absolutely continuous and is given by $\sigma(H_{\text{out}}) = [0,\infty)$ while the spectrum of H_{in} is purely discrete and given by $\sigma(H_{\text{in}}) = \{m^2; m \in \mathbb{N}\}$. Moreover, the sequence of functions $(g_m)_{m\in\mathbb{N}}$ defined on $(0,\pi)$ by

$$g_m(x) = \sqrt{2/\pi}\,\sin(mx) \tag{2.3}$$

is an associated orthonormal basis of eigenfunctions of H_{in}. We also note that $\mathcal{H}_\infty$ can be embedded isometrically in $\mathcal{H}$ via the map $J\colon \mathcal{H}_\infty \to \mathcal{H}$ where for any $\varphi \in \mathcal{H}_\infty$, $J\varphi(x) = \varphi(x)$ if $x \in (0,\pi)\cup(b+\pi,\infty)$ and $J\varphi(x) = 0$ otherwise. Abusing notations, we identify $\mathcal{H}_\infty$ as a subspace of $\mathcal{H}$ in the sequel.

2.2. Energy-time uncertainty principle

We refer to [1] for full details.

Definition 2.1. Let H be a self-adjoint operator on a Hilbert space $\mathcal{H}$ and $\varphi \in \mathcal{H}$. The sojourn time for the state φ with respect to the Hamiltonian H, is defined by:

$$\mathcal{T}(H,\varphi) = \int_{-\infty}^{\infty} |\langle \varphi, e^{-iHt}\varphi\rangle|^2\,dt\,.$$

Definition 2.2. Let H be a self-adjoint operator on a Hilbert space $\mathcal{H}$, $\lambda \in \mathbb{R}$ and $\varphi \in \mathcal{H}\setminus\{0\}$. The energy width $\Delta(H,\varphi,\lambda)$ of the state φ at λ w.r.t the Hamiltonian H is defined as the unique real number:

$$\begin{aligned}\Delta(H,\varphi,\lambda) &= \inf\left\{\epsilon > 0 : \epsilon^2\,\|R(\lambda+i\epsilon)\varphi\|^2 \geq \frac{1}{2}\right\}\\ &= \inf\left\{\epsilon > 0 : 2\epsilon\,\Im\langle\varphi, R(\lambda+i\epsilon)\varphi\rangle \geq 1\right\}\end{aligned}$$

where $R(z) := (H-z)^{-1}$, $z \in \rho(H)$.

The next result is cited from and proven in [1], Theorem 2.5.

Lemma 2.1 (Uncertainty Principle). *Let H be a self-adjoint operator on a Hilbert space $\mathcal{H}$. Then, it holds that for any state $\varphi \in \mathcal{H}$ and any $\lambda \in \mathbb{R}$,*

$$\mathcal{T}(H,\varphi) \geq \Delta(H,\varphi,\lambda)^{-1}\,. \tag{2.4}$$

Further considerations can be found in [1], [5], [9].

2.3. Main result

We follow the notations of the previous sections. Given $(a,m) \in (0,\infty)\times\mathbb{N}$, we denote by $\Delta_{a,m} := \Delta(H_a, g_m, m^2)$ the energy width corresponding to the state g_m at energy m^2. By explicit calculations, the time asymptotic obtained in [3] can be used to prove that there exists a positive constant C, independent of a such that

$$\mathcal{T}(H_a, g_m) \leq C\sqrt{a-m^2}$$

for all $a \geq a_1$ for some $a_1 > m^2$. Here, we construct an explicit upper bound for the energy width, which provides a lower bound for the sojourn time, of the same order.

Theorem 2.1. *Let (H_a) be the family of self-adjoint operators defined by* (2.1). *Then*

(a) $\lim_{a\to\infty} \Delta_{a,m} \sqrt{a-m^2} = \frac{2m^2}{\pi}$,

(b) *there exists a positive constant c, independent of a such that*

$$\mathcal{T}(H_a, g_m) \geq c\sqrt{a-m^2}$$

for all $a \geq a_2$ for some $a_2 > m^2$.

3. Technicalities

3.1. An ODE lemma

In this section we construct and compute the Green function for the differential self-adjoint operator H acting on $\mathcal{H} = L^2_D(0,\infty)$ given by

$$H = -\frac{d^2}{dx^2} + V$$

where V satisfies the following properties:

(C1) V is a real-valued nonnegative function.

(C2) $V \in L^\infty(0,\infty)$.

(C3) V has compact support contained in the interval $[0, \pi + b]$.

Let us denote by ϕ_1, ϕ_2 two linear independent solutions of the eigenvalue problem,

$$-\phi'' + V\phi = k^2\phi\,, \quad x \geq 0, \tag{3.1}$$

where $k^2 = \lambda + i\epsilon$ is a complex number with ϵ, λ real positive numbers.

Following [6], we require that the eigenfunction ϕ_1 satisfies the initial conditions $\phi_1(0) = 0\,, \phi_1'(0) = 1$ while ϕ_2 is chosen in such way that $\phi_2'(x) = ik\phi_2(x)$ for $x > \pi + b$ and such that the Wronskian $W(x) := W(\phi_1, \phi_2)(x) = \phi_1(x)\phi_2'(x) - \phi_1'(x)\phi_2(x) \equiv 1$. Actually, these functions are square integrable for $\Im k$ positive and bounded, for k real (see [6]).

Remark: Following [7], we can also prove that resonances for our problem are located in the lower complex half-plane. Since in our discussion, $\Im k > 0$, we cannot construct a solution to (3.1) which satisfies both the Dirichlet and outgoing conditions. This implies that the functions ϕ_1 and ϕ_2 are a priori linearly independent.

Lemma 3.1. *Let f be an $L^\infty(0,\infty)$ function with compact support. The unique solution of*

$$-\psi'' + V\psi = k^2\psi + f\ , x > 0$$

with $\psi(0) = 0$ and $\psi(x) = c_1 e^{ikx}$ for $|x|$ large, is given by

$$\psi(x) = -\phi_1(x)\int_x^\infty \phi_2(\tau)f(\tau)\,d\tau - \phi_2(x)\int_0^x \phi_1(\tau)f(\tau)\,d\tau. \tag{3.2}$$

Proof. Existence and uniqueness are granted since k is not a scattering frequency ($\Im k > 0$). The representation (3.2) comes from the usual variation of parameter formula and the fact that the Wronskian $W(x) \equiv 1$. □

3.2. Resolvent representation

Throughout this section we assume that $k^2 = \lambda + i\epsilon$ with $\Im k > 0$. Our goal in this section is to study the asymptotic behavior, for a large, of the Fourier transform of the quantity

$$q_m(a,k) = \langle g_m, (H_a - \lambda - i\epsilon)^{-1} g_m \rangle \,, \tag{3.3}$$

where g_m is the eigenfunction of H_∞ defined by (2.3).

Let us denote $f_m = (H_a - k^2)^{-1} g_m$. By Lemma 3.1 and since g_m is supported on $[0,\pi]$ we get that

$$f_m(x) = -\phi_1(x) \int_x^\pi \phi_2(\tau) g_m(\tau)\, d\tau - \phi_2(x) \int_0^x \phi_1(\tau) g_m(\tau)\, d\tau \,. \tag{3.4}$$

First we work out with the factor $\int_x^\pi \phi_2(\tau) g_m(\tau)\, d\tau$.

Clearly, the barrier potential V_a satisfies conditions (C1), (C2) and (C3). Recall that we have chosen two linear independent solutions of the eigenvalue problem (3.1) with $V = V_a$. Using that $-\phi_2'' + V_a \phi_2 = k^2 \phi_2$ we obtain that

$$\begin{aligned}(k^2 - m^2) \int_x^\pi \phi_2(\tau) g_m(\tau)\, d\tau &= \int_x^\pi (g_m''(\tau)\phi_2(\tau) - g_m(\tau)\phi_2''(\tau))\, d\tau \\ &= W(\phi_2, g_m)(\pi) - W(\phi_2, g_m)(x).\end{aligned}$$

A similar argument applies to the second factor, concluding that

$$\begin{aligned}\int_x^\pi \phi_2(\tau) g_m(\tau)\, d\tau &= \frac{1}{k^2 - m^2} \left(W(\phi_2, g_m)(\pi) - W(\phi_2, g_m)(x) \right) \,, \\ \int_0^x \phi_1(\tau) g_m(\tau)\, d\tau &= \frac{1}{k^2 - m^2} W(\phi_1, g_m)(x) \,.\end{aligned}$$

Coming back to the resolvent representation (3.4) together with the above identities, we obtain that

$$\begin{aligned}f_m(x) &= \frac{1}{k^2 - m^2} \left(-\phi_2(\pi) g_m'(\pi) \phi_1(x) - g_m(x) W(\phi_1, \phi_2) \right) \\ &= \frac{1}{k^2 - m^2} \left(-\phi_2(\pi) g_m'(\pi) \phi_1(x) - g_m(x) \right) \,.\end{aligned}$$

We resume the above computations in the following lemma.

Lemma 3.2. *Let H_a be the self-adjoint operator defined by* (2.1) *and $k^2 = \lambda + i\epsilon$ with $\epsilon > 0$ and $\lambda \in \mathbb{R}$. Consider g_m an eigenstate of the limiting self-adjoint operator $H_\infty = H_{\text{in}} \oplus H_{\text{out}}$. Then*

$$f_m(x) = \frac{1}{k^2 - m^2} \left(-\phi_2(\pi) g_m'(\pi) \phi_1(x) - g_m(x) \right) \,. \tag{3.5}$$

As a direct consequence, we have that:

Theorem 3.1. *Let H_a be the self-adjoint operator defined by* (2.1) *and $k^2 = \lambda + i\epsilon$ with $\epsilon > 0$. Consider g_m an eigenstate of the limiting self-adjoint operator $H_\infty = H_{\text{in}} \oplus H_{\text{out}}$. Then*

$$q_m(a,k) = -\frac{1}{k^2 - m^2} - \frac{\phi_2(\pi)g_m'(\pi)}{k^2 - m^2} \int_0^\pi \phi_1(x) g_m(x) dx\,. \tag{3.6}$$

Since the eigenfunction ϕ_1 is explicitly known inside the barrier, we only need to estimate the coefficient $\phi_2(\pi)$, in terms of the height a of the barrier V_a.

We now proceed to construct two linear independent eigenfunctions, ϕ_1, ϕ_2 of the operator (3.1) satisfying that $\phi_1(0) = 0, \phi_1'(0) = 1$, $\phi_2' = ik\phi_2$ for $x > \pi + b$ and $W(\phi_1, \phi_2) = 1$.

We start by building a function $\psi \in L^2_D(0,\infty)$ such that $-\psi'' + V_a(x)\psi = k^2\psi$ for $x > 0$. First, we choose

$$\psi(x) = e^{ikx} \quad \text{for} \quad x > \pi + b\,.$$

For $\pi < x < \pi + b$, the equation reads $-\psi'' = (k^2 - a)\psi$ and, by matching the boundary conditions at $\pi + b$, we have that inside the barrier ψ is given by

$$\psi(x) = \frac{e^{ik(\pi+b)}}{2a_k} \left((a_k + ik) e^{-a_k(\pi+b)} e^{a_k x} + (a_k - ik) e^{a_k(\pi+b)} e^{-a_k x} \right) \tag{3.7}$$

where $a_k = \sqrt{a - k^2}$. Notice that the L^2 property is guaranteed by the condition $\Im k > 0$. We notice that as a becomes large, $\Re a_k > 0$.

Next, we proceed by extending the solutions to the region $0 < x < \pi$, where the equation becomes $-\psi'' = k^2\psi$. Applying a similar argument we conclude that

$$\psi(x) = \frac{ik\psi(\pi) + \psi'(\pi)}{2ik} e^{-ik\pi} e^{ikx} + \frac{ik\psi(\pi) - \psi'(\pi)}{2ik} e^{ik\pi} e^{-ikx} \tag{3.8}$$

for $0 < x < \pi$ where $\psi(\pi), \psi'(\pi)$ are given by (3.7).

Lemma 3.3. *Consider $k^2 = \lambda + i\epsilon$. For the potential barrier V_a given by* (2.2) *there exist two linearly independent eigenfunctions, ϕ_1, ϕ_2 of the operator* (3.1) *satisfying the conditions: $\phi_1(0) = 0, \phi_1'(0) = 1$ and $\phi_2' = ik\phi_2$ for $x > \pi + b$ with $W(\phi_1, \phi_2) = 1$. In addition we have that*

$$\phi_2(\pi) = -\frac{2ik}{B(k)} \left(\frac{\psi'(\pi)}{\psi(\pi)} + ik\frac{A(k)}{B(k)} \right)^{-1}, \tag{3.9}$$

with $a_k = \sqrt{a - k^2}$, $A(k) = e^{-ik\pi} + e^{ik\pi}$ and $B(k) = e^{-ik\pi} - e^{ik\pi}$.

Proof. Notice that for a large enough, $\psi(0) \neq 0$ where ψ is the extension defined by (3.8). Now, we choose $\phi_2(x) = -\frac{1}{\psi(0)}\psi(x)$. Clearly, $W(\phi_1, \phi_2) = 1$ and $\phi_2(\pi) = -\frac{1}{\psi(0)}\psi(\pi)$. By evaluating (3.8) at $x = 0$,

$$\frac{\psi(0)}{\psi(\pi)} = \frac{1}{2}\left(e^{-ik\pi} + e^{ik\pi}\right) + \frac{\psi'(\pi)}{\psi(\pi)} \frac{1}{2ik}\left(e^{-ik\pi} - e^{ik\pi}\right)\,.$$

From the above identity we conclude (3.9), thus ending the proof. □

3.3. Proof of Theorem 2.1

Proof. It is easy to compute that

$$\int_0^\pi \phi_1(x) g_m(x)\, dx = \frac{1}{k^2 - m^2}\,(\phi_1(\pi) g_m'(\pi)).$$

Thus, (3.6) becomes

$$\langle g_m, (H_a - \lambda - i\epsilon)^{-1} g_m\rangle = -\frac{1}{k^2 - m^2} - \frac{2m^2}{\pi(k^2 - m^2)^2}\,\phi_1(\pi)\phi_2(\pi).$$

By taking $\lambda = m^2$ we deduce that the corresponding imaginary part of this quadratic form is given by

$$\Im\langle g_m, (H_a - m^2 - i\epsilon)^{-1} g_m\rangle = \frac{1}{\epsilon} + \frac{2m^2}{\pi\epsilon^2}\,\Im(\phi_1(\pi)\phi_2(\pi))\,. \tag{3.10}$$

Next, by using the definition of the energy width, identity (3.10) and by choosing $\epsilon = \Delta_{a,m} > 0$, we deduce that

$$\frac{1}{2} = \epsilon\, \Im\left(\langle g_m, (H_a - m^2 - i\epsilon)^{-1} g_m\rangle\right) = 1 + \frac{2m^2}{\pi\Delta_{a,m}}\Im(\phi_1(\pi)\phi_2(\pi)) \tag{3.11}$$

where $\Delta_{a,m}$ is the energy width, $\Delta_{a,m} = \Delta(H_a, g_m, m^2)$.

This proves that

$$\Delta_{a,m} = -\frac{4m^2}{\pi}\,\Im(\phi_1(\pi)\phi_2(\pi))\,.$$

The generalized eigenfunction ϕ_1 is explicit in the interval $[0,\pi]$, indeed $\phi_1(\pi) = -\frac{B(k)}{2ik}$. By using this and the representation of ϕ_2, we conclude

$$\phi_1(\pi)\phi_2(\pi) = \frac{1}{\frac{\psi'(\pi)}{\psi(\pi)} + ik\frac{A(k)}{B(k)}}\,,$$

where the auxiliary function ψ is given by equation (3.7) in the interval $[\pi, \pi + b]$.

Here, $A(k)$ and $B(k)$ are given in Lemma 3.3 and $k^2 = m^2 + i\epsilon$.

Thus, the energy width at the unperturbed eigenfunction g_m satisfies

$$\Delta_{a,m} = -\frac{4m^2}{\pi}\,\Im\left(\frac{1}{\frac{\psi'(\pi)}{\psi(\pi)} + ik\frac{A(k)}{B(k)}}\right)\,. \tag{3.12}$$

When a tends to infinity, both terms in the denominator inside the imaginary part of this expression approach infinity.

By (3.7), the first of these terms is

$$\frac{\psi'(\pi)}{\psi(\pi)} = a_k\frac{(a_k + ik)e^{-a_k b} - (a_k - ik)e^{a_k b}}{(a_k + ik)e^{-a_k b} + (a_k - ik)e^{a_k b}}\,, \tag{3.13}$$

where $a_k = \sqrt{a - k^2}$.

On the other hand, since the operator H_a converges in the strong resolvent sense to H_∞, we have that as $a \to \infty$, the energy width $\epsilon = \Delta_{a,m}$ converges to zero. This fact also follows directly from the equation (3.12), by multiplying both sides by $\sqrt{a-m^2}$ and computing the limit when $a \to \infty$.

A direct computation gives that for a large and hence, ϵ small,

$$B(k) = \frac{\pi}{m}\epsilon - \frac{\pi}{4m^3}\epsilon^2 + O(\epsilon^3)\,.$$

Also,

$$A(k) = 2 - \frac{\pi^2}{2m}\epsilon^2 + O(\epsilon^3)\,.$$

Therefore, equation (3.12) gives

$$\Delta_{a,m} = -\frac{4m^2}{\pi}\Im\left(a_k c_k + ik\frac{2-\frac{\pi^2}{2m}\epsilon^2+O(\epsilon^3)}{\frac{\pi}{m}\epsilon - \frac{\pi}{4m^3}\epsilon^2 + O(\epsilon^3)}\right)^{-1},$$

where

$$c_k = \frac{(a_k+ik)e^{-a_k b} - (a_k-ik)e^{a_k b}}{(a_k+ik)e^{-a_k b} + (a_k-ik)e^{a_k b}}\,. \tag{3.14}$$

We finally divide both sides by $\epsilon = \Delta_{a,m}$ to obtain

$$1 = -\frac{4m^2}{\pi}\Im\left(\epsilon a_k c_k + ik\frac{2-\frac{\pi^2}{2m}\epsilon^2+O(\epsilon^3)}{\frac{\pi}{m} - \frac{\pi}{4m^3}\epsilon + O(\epsilon^2)}\right)^{-1}.$$

From the formula (3.14), we deduce that $c_k \to -1$, as $a \to \infty$. Hence,

$$L := \lim_{a\to\infty} a_k\epsilon$$

exists and it satisfies

$$1 = -\frac{4m^2}{\pi}\Im\left(\frac{1}{-L + i\frac{2m^2}{\pi}}\right).$$

This gives

$$L = \lim_{a\to\infty} a_k\epsilon = \frac{2m^2}{\pi}\,.$$

Part (a) follows from the fact that $\lim_{a\to\infty} a_k(a-m^2)^{-1} = 1$ and we conclude the estimate (b) from the uncertainty principle Lemma 2.1. □

We remark that while we used formula (3.12) to estimate the asymptotic behaviour of the energy width, as a diverges, the formula could also be used to obtain an asymptotic expansion and thus a more precise lower bound for the sojourn time.

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Spectral Properties for Hamiltonians of Weak Interactions

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Abstract. We present recent results on the spectral theory for Hamiltonians of the weak decay. We discuss rigorous results on self-adjointness, location of the essential spectrum, existence of a ground state, purely absolutely continuous spectrum and limiting absorption principles. The last two properties heavily rely on the so-called Mourre Theory, which is used, depending on the Hamiltonian we study, either in its standard form, or in a more general framework using non self-adjoint conjugate operators.

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1. Introduction

We study various mathematical models for the weak interactions that can be patterned according to the Standard Model of Quantum Field Theory. The reader may consult [30, (4.139)] and [50, (21.3.20)]) for a complete description of the physical Lagrangian of the lepton-gauge boson coupling. A full mathematical understanding of spectral properties for the associated Hamiltonians is not yet achieved, and a rigorous description of the dynamics of particles remains a tremendous task. It is however possible to obtain relevant results in certain cases, like for example a characterization of the absolutely continuous spectrum and limiting absorption principles. One of the main obstacles is to be able to establish rigorous results without denaturing the original (ill-defined) physical Hamiltonians, by imposing only mathematical mild and physically interpretable additional assumptions. Among other technical difficulties carried by each models, there are two common problems. A basic one is to prove that the interaction part of the Hamiltonian is relatively bounded with respect to the free Hamiltonian. Without this basic property, it is in general rather illusory to prove more than self-adjointness for the energy operator. This question can be reduced to the adaptation of the N_τ estimates of Glimm and Jaffe [21], as done, e.g., in [8], with however serious difficulties for processes involving more than four particles or more than one massless particle. Another major difficulty is to prove a limiting absorption principle without imposing any infrared regularization. This problem can be partly overcome at the expense of a careful study of the Dirac and Boson fields, and thus a study of local properties for the generalized solutions to various partial differential equations, like, e.g., the Dirac equations with or without external fields, or the Proca equation.

Derivation of spectral properties for weak interactions – or very similar – models have been achieved in [7, 8, 2, 22, 11, 13, 26, 4, 9, 10, 32, 33]. In the present article, we present a review of the results of [2, 11, 13, 32, 4, 9], focusing on two different processes, one for the gauge bosons $W^{\pm}$ and one for the gauge boson Z^0. These models already catch some of the main mathematical difficulties encountered in the above-mentioned works. The first model is the decay of the intermediate vector bosons $W^{\pm}$ into the full family of leptons. The second is the decay of the vector boson Z^0 into pairs of electrons and positrons. Both processes involve only three different kind of particles, two fermions and one boson. However, they have a fundamental difference. The first one involves *massless* particles whereas the second one has only *massive* particles. This forces us to use rather different strategies to attack the study of spectral properties.

First model: In the weak decay of the intermediate vector bosons $W^{\pm}$ into the full family of leptons, the involved particles are the electron e^- and its antiparticle, the positron e^+, together with the associated neutrino ν_e and antineutrino $\bar{\nu}_e$, the muons μ^- and μ^+ together with the associated neutrino ν_μ and antineutrino $\bar{\nu}_\mu$ and the tau leptons τ^- and τ^+ together with the associated neutrino ν_τ and antineutrino $\bar{\nu}_\tau$.

A representative and well-known example of this general process is the decay of the gauge boson W^- into an electron and an antineutrino of the electron that occurs in the β-decay that led Pauli to conjecture the existence of the neutrino [39]

$$W^- \to e^- + \bar{\nu}_e .$$

For the sake of clarity, we shall stick to this case in the first model. The general situation with all other leptons can be recovered in a straightforward way.

The interaction for this $W^{\pm}$ decay, described in the Schrödinger representation, is formally given by (see [30, (4.139)] and [50, (21.3.20)])

$$I_{W^{\pm}} = \int \overline{\Psi_e}(x)\gamma^\alpha(1-\gamma_5)\Psi_{\nu_e}(x)W_\alpha(x)\mathrm{d}x + \int \overline{\Psi_{\nu_e}}(x)\gamma^\alpha(1-\gamma_5)\Psi_e(x)W_\alpha(x)^*\mathrm{d}x ,$$

where γ^α, $\alpha = 0,1,2,3$, and γ_5 are the Dirac matrices, $\Psi_.(x)$ and $\overline{\Psi_.}(x)$ are the Dirac fields for $e_\pm$, ν_e, and $\bar{\nu}_e$, and W_α are the boson fields (see [49, §5.3] and Section 2).

If one formally expands this interaction with respect to products of creation and annihilation operators, we are left with a finite sum of terms associated with kernels of the form

$$\delta(p_1 + p_2 - k)g(p_1,\ p_2,\ k) \ ,$$

with $g \in L^1$. Our restriction here only consists in approximating these kernels by square integrable functions with respect to momenta (see (2.3) and (2.4)–(2.6)).

Under this assumption, the total Hamiltonian, which is the sum of the free energy of the particles (see (2.2)) and of the interaction, is a well-defined self-adjoint operator (Theorem 2.2).

In addition, we can show (Theorem 2.6) that for a sufficiently small coupling constant, the total Hamiltonian has a unique ground state corresponding to the dressed vacuum. This property is not obvious since usual Kato's perturbation theory does not work here due to the fact that according to the standard model, neutrinos are massless particles (see discussion in Section 2), thus the unperturbed hamiltonian, namely the full Hamiltonian where the interaction between the different particles has been turned off, has a ground state with energy located at the bottom of the essential spectrum. The strategy for proving existence of a unique ground state for similar models has its origin in the seminal works of Bach, Fröhlich, and Sigal [6] (see also [40], [5] and [31]), for the Pauli–Fierz model of non-relativistic QED. Our proofs follow these techniques as adapted in [7, 8, 17] to a model of quantum electrodynamics and in [2] to a model of the Fermi weak interactions.

Under natural regularity assumptions on the kernels, we next establish a Mourre estimate (Theorem 2.8) and a limiting absorption principle (Theorem 2.10) for any spectral interval down to the energy of the ground state and below the mass of the electron, for small enough coupling constants. As a consequence, the whole spectrum between the ground state and the first threshold is shown to be purely absolutely continuous (Theorem 2.7).

Our method to achieve the spectral analysis above the ground state energy, follows [5, 19, 14], and is based on the proof of a spectral gap property for Hamiltonians with a cutoff interaction for small neutrino momenta and acting on neutrinos of strictly positive energies.

Eventually, as in [19, 13, 14], we use this gap property in combination with the conjugate operator method developed in [3] and [44] in order to establish a limiting absorption principle near the ground state energy of H_W. In [13], the chosen conjugate operator was the generator of dilatations in the Fock space for neutrinos and antineutrinos. As a consequence, an infrared regularization was assumed in [13] in order to be able to implement the strategy of [19]. To overcome this difficulty and avoid infrared regularization, we choose in [4] a conjugate operator which is the generator of dilatations in the Fock space for neutrinos and antineutrinos *with a cutoff in the momentum variable*. Our conjugate operator thus only affects the massless particles of low energies. A similar choice is made in [14] for a model of non-relativistic QED for a free electron at fixed total momentum. Compared with [19] and [14], our method involves further estimates, which allows us to avoid any infrared regularization. Under stronger assumptions, the model of $W^{\pm}$ decay has been studied in [7, 13]. We present in Section 2 the results obtained in [4], where the main achievement is that no infrared regularization is assumed.

Second Model: The physical phenomenon in the decay of the gauge boson we consider here only involves *massive* particles, the massive boson Z^0, electrons and positrons,

$$Z^0 \to e^- + e^+ .$$

In some respects, e.g., as far as the existence of a ground state is concerned, this feature renders trivial the spectral analysis of the Hamiltonian. On the other hand, due to the positive masses of the particles, an infinite number of thresholds occur in the spectrum of the unperturbed Hamiltonian. Understanding the nature of the spectrum of the full Hamiltonian near the thresholds as the interaction is turned on then becomes a subtle question, as it is known that spectral analysis near thresholds, in particular by means of perturbation theory, is a delicate subject. This question is the main concern in the analysis of the second model.

The interaction between the electrons, positrons and the boson vectors Z^0, in the Schrödinger representation, is given, up to coupling constants, by (see [30, (4.139)] and [50, (21.3.20)])

$$I_{Z^0} = \int \overline{\Psi_e}(x)\gamma^\alpha(g'_V - \gamma_5)\Psi_e(x) Z_\alpha(x)\,\mathrm{d}x + h.c., \tag{1.1}$$

where, as above, γ^α, $\alpha = 0,1,2,3$, and γ_5 are the Dirac matrices and $\Psi_e(x)$ and $\overline{\Psi_e}(x)$ are the Dirac fields for the electron e^- and the positron e^+ of mass m_e. The field Z_α is the massive boson field for Z^0. The constant g'_V is a real parameter such that $g'_V \simeq 0,074$ (see, e.g., [30]).

The main results provide a complete description of the spectrum of the Hamiltonian below the boson mass. We will show that the spectrum is composed of a unique isolated eigenvalue E, the ground state energy corresponding to the dressed vacuum, and the semi-axis of essential spectrum $[E+\mathrm{m}_e, \infty)$, m_e being the electron mass (Theorem 3.4).

Moreover, with mild regularity assumptions on the kernel, using a version of Mourre's theory allowing for a non self-adjoint conjugate operator and requiring only low regularity of the Hamiltonian with respect to this conjugate operator, we establish a limiting absorption principle and prove that the essential spectrum below the boson mass is purely absolutely continuous (Theorem 3.5).

In order to establish these results, we need to use a spectral representation of the self-adjoint Dirac operator generated by a sequence of spherical waves (see [29] and Section 3). If we have been using the plane waves as for the first model above, for example the four ones associated with the helicity (see [47]), the two kernels $G^{(\alpha)}(\cdot)$ of the interaction would have had to satisfy an infrared regularization with respect to the fermionic variables. By our choice of the sequence of the spherical waves, our analysis only requires that the kernels of the interaction satisfy an infrared regularization for two values of the discrete parameters characterizing the sequence of spherical waves. For any other value of the discrete parameters, we do not need to introduce an infrared regularization.

The article is organized as follows. Section 2 is devoted to the study of the first model, the decay of the gauge bosons W^- into an electron and its associated neutrino. The first part contains a detailed construction of the Fock Hilbert spaces and the mathematical Hamiltonian for the decay. The second part of Section 2 deals with the central results of the spectral analysis for this Hamiltonian, as well as some steps of a proof for the limiting absorption principle. All details can be found in [4]. Section 3 is concerned with the decay of the gauge bosons Z^0 into electrons and positrons. There, we also give a detailed description of Hilbert spaces, notably different than in the previous section due to the writing of the Dirac fields with spherical waves. We also write a construction of the Hamiltonian for the decay of the Z^0 boson. We subsequently present the main theorems on spectral and dynamical properties, with some hints concerning the proof of the limiting absorption principle. All details can be found in [9]. Section 4 is devoted to a short presentation of open questions and ongoing work; whenever it is possible we point out the mathematical difficulties for these new problems.

2. Interaction of the Gauge boson $W^\pm$ with an electron and a massless neutrino

According to the Standard Model, the weak decay of the intermediate bosons W^+ and W^- involves the full family of leptons: electrons, muons, tauons, their associated neutrinos and the corresponding antiparticles (see [30, Formula (4.139)] and [50]). In the Standard Model, neutrinos and antineutrinos are assumed to be massless. Despite experimental evidences [20] that in fact neutrinos have a mass, an extended version of the Standard Model to account for this mass is beyond the scope of this article.

Neutrinos and antineutrinos are particles with helicity $-1/2$ and $+1/2$, respectively. Here we shall assume that both neutrinos and antineutrinos have helicity $\pm 1/2$.

As already mentioned in the introduction, without loss of generality, we restrict ourselves to the decay of the gauge boson W^- into an electron and an antineutrino,

$$W^- \to e^- + \bar{\nu}_e. \tag{2.1}$$

However, all results remain true if we consider instead the decay of the $W^\pm$ into the full family of leptons.

If we include the corresponding antiparticles in the process (2.1), the interaction described in the Schrödinger representation is formally given by (see [30, (4.139)] and [50, (21.3.20)])

$$I_{W^\pm} = \int_{\mathbb{R}^3} \overline{\Psi_e}(x)\gamma^\alpha(1-\gamma_5)\Psi_{\nu_e}(x)W_\alpha(x)\mathrm{d}x + \int_{\mathbb{R}^3} \overline{\Psi_{\nu_e}}(x)\gamma^\alpha(1-\gamma_5)\Psi_e(x)W_\alpha(x)^*\mathrm{d}x,$$

where γ^α, $\alpha = 0,1,2,3$, and γ_5 are the Dirac matrices, $\Psi_\cdot(x)$ and $\overline{\Psi_\cdot}(x)$ are the Dirac fields for $e_\pm$, ν_e, and $\bar{\nu}_e$, and W_α are the boson fields (see [49, §5.3]) given respectively by

$$\Psi_e(x) = (2\pi)^{-\frac{3}{2}} \sum_{s=\pm\frac{1}{2}} \int_{\mathbb{R}^3} \Big(\frac{u(p,s)}{(2(|p|^2+\mathrm{m}_e{}^2)^{\frac{1}{2}})^{\frac{1}{2}}}\, b_+(p,s)\mathrm{e}^{ip.x} + \frac{v(p,s)}{(2(|p|^2+\mathrm{m}_e{}^2)^{\frac{1}{2}})^{\frac{1}{2}}}\, b_-^*(p,s)\mathrm{e}^{-ip.x}\Big)\mathrm{d}p,$$

$$\Psi_{\nu_e}(x) = (2\pi)^{-\frac{3}{2}} \sum_{s=\pm\frac{1}{2}} \int_{\mathbb{R}^3} \Big(\frac{u(p,s)}{(2|p|)^{\frac{1}{2}}}\, c_+(p,s)\mathrm{e}^{ip.x} + \frac{v(p,s)}{(2|p|)^{\frac{1}{2}}}\, c_-^*(p,s)\mathrm{e}^{-ip.x}\Big)\mathrm{d}p\,,$$

$$\overline{\Psi_e}(x) = \Psi_e(x)^\dagger\gamma^0\,, \quad \overline{\Psi_{\nu_e}}(x) = \Psi_{\nu_e}(x)^\dagger\gamma^0\,,$$

and

$$W_\alpha(x) = (2\pi)^{-\frac{3}{2}} \sum_{\lambda=-1,0,1} \int_{\mathbb{R}^3} \Big(\frac{\epsilon_\alpha(k,\lambda)}{(2(|k|^2+\mathrm{m}_W{}^2)^{\frac{1}{2}})^{\frac{1}{2}}} a_+(k,\lambda)\mathrm{e}^{ik.x} + \frac{\epsilon_\alpha^*(k,\lambda)}{(2(|k|^2+\mathrm{m}_W{}^2)^{\frac{1}{2}})^{\frac{1}{2}}} a_-^*(k,\lambda)\mathrm{e}^{-ik.x}\Big)\mathrm{d}k\,.$$

Here $\mathrm{m}_e > 0$ is the mass of the electron and $u(p,s)/(2(|p|^2+\mathrm{m}_e{}^2)^{1/2})^{1/2}$ and $v(p,s)/(2(|p|^2+\mathrm{m}_e{}^2)^{1/2})^{1/2}$ are the normalized solutions to the Dirac equation (see for example [30, Appendix]), where $p \in \mathbb{R}^3$ is the momentum variable of the electron, or its antiparticle, and s is its spin. The mass of the bosons $W^\pm$ is denoted by m_W, and fulfills $\mathrm{m}_W > \mathrm{m}_e$ ($\mathrm{m}_W/\mathrm{m}_e \approx 1.57\times 10^5$). The vectors $\epsilon_\alpha(k,\lambda)$ are the polarizations of the massive spin 1 bosons (see [49, Section 5.2]), and as follows from the Standard Model, neutrinos and antineutrinos are considered here to be massless particles.

The operators $b_+(p,s)$ and $b_+^*(p,s)$ (respectively $c_+(p,s)$ and $c_+^*(p,s)$), are the annihilation and creation operators for the electrons (respectively for the neutrinos associated with the electrons), satisfying the anticommutation relations. The index $-$ in $b_-(p,s)$, $b_-^*(p,s)$, $c_-(p,s)$ and $c_-^*(p,s)$ are used to denote the annihilation and creation operators of the corresponding antiparticles. The operators $a_+(k,\lambda)$ and $a_+^*(k,\lambda)$ (respectively $a_-(k,\lambda)$ and $a_-^*(k,\lambda)$) are the annihilation and creation operators for the bosons W^- (respectively W^+) satisfying the canonical commutation relations. The definition of these operators is very standard (see, e.g., [49] or [12]).

2.1. Rigorous definition of the model

The mathematical model for the weak decay of the vector bosons $W^\pm$ is defined as follows.

Let $\xi_1 = (p_1,\ s_1)$ be the quantum variable of a massive lepton, electron or positron, where $p_1 \in \mathbb{R}^3$ is the momentum and $s_1 \in \{-1/2,\ 1/2\}$ is the spin. Let $\xi_2 = (p_2,\ s_2)$ be the quantum variables of a massless neutrino or antineutrino, where $p_2 \in \mathbb{R}^3$ and $s_2 \in \{-1/2,\ 1/2\}$ is the helicity of particles and antiparticles, and, finally, let $\xi_3 = (k,\ \lambda)$ be the quantum variables of the spin 1 bosons W^+ and

W^-, with momenta $k \in \mathbb{R}^3$ and where $\lambda \in \{-1,\ 0,\ 1\}$ accounts for the polarization of the vector bosons (see [49, Section 5.2]).

We define $\Sigma_1 = \mathbb{R}^3 \times \{-1/2,\ 1/2\}$ for the configuration space of the leptons and $\Sigma_2 = \mathbb{R}^3 \times \{-1,\ 0,\ 1\}$ for the bosons. Thus $L^2(\Sigma_1)$ is the one particle Hilbert space of each lepton of this process (electron, positron, neutrino and antineutrino of the electron) and $L^2(\Sigma_2)$ is the one particle Hilbert space of each boson. In the sequel, we shall use the notations $\int_{\Sigma_1} \mathrm{d}\xi := \sum_{s=+\frac{1}{2},-\frac{1}{2}} \int \mathrm{d}p$ and $\int_{\Sigma_2} \mathrm{d}\xi := \sum_{\lambda=0,1,-1} \int \mathrm{d}k$.

The Hilbert space for the weak decay of the vector bosons $W^{\pm}$ is the Fock space for leptons and bosons describing the set of states with indefinite number of particles or antiparticles which we define below.

The space $\mathfrak{F}_L$ is the fermionic Fock space for the massive electron and positron with the associated neutrino and antineutrino, i.e.,

$$\mathfrak{F}_L = \bigotimes^4 \mathfrak{F}_a(L^2(\Sigma_1)) = \bigotimes^4 \left(\oplus_{n=0}^{\infty} \otimes_a^n L^2(\Sigma_1)\right) ,$$

where $\otimes_a^n$ denotes the antisymmetric nth tensor product and $\otimes_a^0 L^2(\Sigma_1) := \mathbb{C}$.

The bosonic Fock space $\mathfrak{F}_W$ for the vector bosons W^+ and W^- reads

$$\mathfrak{F}_W = \bigotimes^2 \mathfrak{F}_s(L^2(\Sigma_2)) = \bigotimes^2 \left(\oplus_{n=0}^{\infty} \otimes_s^n L^2(\Sigma_2)\right) ,$$

where $\otimes_s^n$ denotes the symmetric nth tensor product and $\otimes_s^0 L^2(\Sigma_2) := \mathbb{C}$.

The Fock space for the weak decay of the vector bosons W^+ and W^- is thus

$$\mathfrak{F} = \mathfrak{F}_L \otimes \mathfrak{F}_W .$$

Furthermore, $b_\epsilon(\xi_1)$ (resp. $b_\epsilon^*(\xi_1)$) is the annihilation (resp. creation) operator for the corresponding species of massive particle if $\epsilon = +$ and for the corresponding species of massive antiparticle if $\epsilon = -$. Similarly, $c_\epsilon(\xi_2)$ (resp. $c_\epsilon^*(\xi_2)$) is the annihilation (resp. creation) operator for the corresponding species of neutrino if $\epsilon = +$ and for the corresponding species of antineutrino if $\epsilon = -$. Finally, the operator $a_\epsilon(\xi_3)$ (resp. $a_\epsilon^*(\xi_3)$) is the annihilation (resp. creation) operator for the boson W^- if $\epsilon = +$, and for the boson W^+ if $\epsilon = -$. The operators $b_\epsilon(\xi_1)$, $b_\epsilon^*(\xi_1)$, $c_\epsilon(\xi_2)$, and $c_\epsilon^*(\xi_2)$ fulfil the usual canonical anticommutation relations (CAR), whereas $a_\epsilon(\xi_3)$ and $a_\epsilon^*(\xi_3)$ fulfil the canonical commutation relation (CCR), see, e.g., [49]. Moreover, the a's commute with the b's and the c's. In addition, following the convention described in [49, Section 4.1] and [49, Section 4.2], we will assume that fermionic creation and annihilation operators of different species of leptons anticommute (see, e.g., [12] for an explicit definition involving this additional requirement). Therefore, the following canonical anticommutation and commutation relations hold,

$$\begin{aligned}
&\{b_\epsilon(\xi_1), b^*_{\epsilon'}(\xi'_1)\} = \delta_{\epsilon\epsilon'}\delta(\xi_1 - \xi'_1)\ , \quad \{c_\epsilon(\xi_2), c^*_{\epsilon'}(\xi'_2)\} = \delta_{\epsilon\epsilon'}\delta(\xi_2 - \xi'_2)\ ,\\
&[a_\epsilon(\xi_3), a^*_{\epsilon'}(\xi'_3)] = \delta_{\epsilon\epsilon'}\delta(\xi_3 - \xi'_3)\ ,\\
&\{b_\epsilon(\xi_1), b_{\epsilon'}(\xi'_1)\} = \{c_\epsilon(\xi_2), c_{\epsilon'}(\xi'_2)\} = 0\ ,\\
&[a_\epsilon(\xi_3), a_{\epsilon'}(\xi'_3)] = 0\ ,\\
&\{b_\epsilon(\xi_1), c_{\epsilon'}(\xi_2)\} = \{b_\epsilon(\xi_1), c^*_{\epsilon'}(\xi_2)\} = 0\ ,\\
&[b_\epsilon(\xi_1), a_{\epsilon'}(\xi_3)] = [b_\epsilon(\xi_1), a^*_{\epsilon'}(\xi_3)] = [c_\epsilon(\xi_2), a_{\epsilon'}(\xi_3)] = [c_\epsilon(\xi_2), a^*_{\epsilon'}(\xi_3)] = 0\ ,
\end{aligned}$$

where $\{b, b'\} = bb' + b'b$ and $[a, a'] = aa' - a'a$. For $\varphi \in L^2(\Sigma_1)$, the operators

$$\begin{aligned}
b_\epsilon(\varphi) &= \int_{\Sigma_1} b_\epsilon(\xi)\overline{\varphi(\xi)}\mathrm{d}\xi, \quad c_\epsilon(\varphi) = \int_{\Sigma_1} c_\epsilon(\xi)\overline{\varphi(\xi)}\mathrm{d}\xi\ ,\\
b^*_\epsilon(\varphi) &= \int_{\Sigma_1} b^*_\epsilon(\xi)\varphi(\xi)\mathrm{d}\xi, \quad c^*_\epsilon(\varphi) = \int_{\Sigma_1} c^*_\epsilon(\xi)\varphi(\xi)\mathrm{d}\xi\ ,
\end{aligned}$$

are bounded operators on $\mathfrak{F}$ satisfying $\|b^\sharp_\epsilon(\varphi)\| = \|c^\sharp_\epsilon(\varphi)\| = \|\varphi\|_{L^2}$, where $b^\sharp$ (resp. $c^\sharp$) is b (resp. c) or b^* (resp. c^*).

The free Hamiltonian $H_{W,0}$ is given by

$$\begin{aligned}
H_{W,0} = \sum_{\epsilon=\pm}\int w^{(1)}(\xi_1)b^*_\epsilon(\xi_1)b_\epsilon(\xi_1)\mathrm{d}\xi_1 + \sum_{\epsilon=\pm}\int w^{(2)}(\xi_2)c^*_\epsilon(\xi_2)c_\epsilon(\xi_2)\mathrm{d}\xi_2\\
+ \sum_{\epsilon=\pm}\int w^{(3)}(\xi_3)a^*_\epsilon(\xi_3)a_\epsilon(\xi_3)\mathrm{d}\xi_3\ ,
\end{aligned} \tag{2.2}$$

where the free relativistic energy of the massive leptons, the neutrinos, and the bosons are respectively given by

$$w^{(1)}(\xi_1) = (|p_1|^2 + \mathrm{m}_e{}^2)^{\frac{1}{2}},\ w^{(2)}(\xi_2) = |p_2|, \text{ and } w^{(3)}(\xi_3) = (|k|^2 + \mathrm{m}_W{}^2)^{\frac{1}{2}}\ .$$

The interaction $H_{W,I}$ is described in terms of annihilation and creation operators together with kernels $G^{(\alpha)}_{\epsilon,\epsilon'}(.,.,.)$ $(\alpha = 1, 2)$.

As emphasized in the introduction, each kernel $G^{(\alpha)}_{\epsilon,\epsilon'}(\xi_1, \xi_2, \xi_3)$, computed in theoretical physics, contains a δ-distribution because of the conservation of the momentum (see [30], [49, Section 4.4]). Here, we approximate the singular kernels by square integrable functions. Therefore, we assume the following

Hypothesis 2.1. *For $\alpha = 1, 2$, $\epsilon, \epsilon' = \pm$, we assume*

$$G^{(\alpha)}_{\epsilon,\epsilon'}(\xi_1, \xi_2, \xi_3) \in L^2(\Sigma_1 \times \Sigma_1 \times \Sigma_2)\ . \tag{2.3}$$

Based on [30, p. 159, (4.139)] and [50, p. 308, (21.3.20)], we define the interaction as

$$H_{W,I} = H^{(1)}_{W,I} + H^{(2)}_{W,I}\ , \tag{2.4}$$

where

$$
\begin{aligned}
H^{(1)}_{W,I} = & \sum_{\epsilon\neq\epsilon'} \int G^{(1)}_{\epsilon,\epsilon'}(\xi_1,\xi_2,\xi_3) b^*_\epsilon(\xi_1) c^*_{\epsilon'}(\xi_2) a_\epsilon(\xi_3)\, \mathrm{d}\xi_1 \mathrm{d}\xi_2 \mathrm{d}\xi_3 \\
& + \sum_{\epsilon\neq\epsilon'} \int \overline{G^{(1)}_{\epsilon,\epsilon'}(\xi_1,\xi_2,\xi_3)} a^*_\epsilon(\xi_3) c_{\epsilon'}(\xi_2) b_\epsilon(\xi_1)\, \mathrm{d}\xi_1 \mathrm{d}\xi_2 \mathrm{d}\xi_3 \ ,
\end{aligned}
\tag{2.5}
$$

$$
\begin{aligned}
H^{(2)}_{W,I} = & \sum_{\epsilon\neq\epsilon'} \int G^{(2)}_{\epsilon,\epsilon'}(\xi_1,\xi_2,\xi_3) b^*_\epsilon(\xi_1) c^*_{\epsilon'}(\xi_2) a^*_\epsilon(\xi_3) \mathrm{d}\xi_1 \mathrm{d}\xi_2 \mathrm{d}\xi_3 \\
& + \sum_{\epsilon\neq\epsilon'} \int \overline{G^{(2)}_{\epsilon,\epsilon'}(\xi_1,\xi_2,\xi_3)} a_\epsilon(\xi_3) c_{\epsilon'}(\xi_2) b_\epsilon(\xi_1)\, \mathrm{d}\xi_1 \mathrm{d}\xi_2 \mathrm{d}\xi_3 \ .
\end{aligned}
\tag{2.6}
$$

The operator $H^{(1)}_{W,I}$ describes the decay of the bosons W^+ and W^- into leptons, and $H^{(2)}_{W,I}$ is responsible for the fact that the bare vacuum will not be an eigenvector of the total Hamiltonian, as expected from physics.

All terms in $H^{(1)}_{W,I}$ and $H^{(2)}_{W,I}$ are well defined as quadratic forms on the set of finite particle states consisting of smooth wave functions. According to [41, Theorem X.24] (see details in [13]), one can construct a closed operator associated with the quadratic form defined by (2.4)–(2.6).

The total Hamiltonian is thus ($g \in \mathbb{R}$ is a coupling constant),

$$H_W = H_{W,0} + gH_{W,I}.$$

2.2. Limiting absorption principle and spectral properties

We begin with a basic self-adjointness property.

Theorem 2.2 (Self-adjointness). *Let $g_1 > 0$ be such that*

$$\frac{6g_1^2}{\mathrm{m}_W}\left(\frac{1}{\mathrm{m}_e{}^2}+1\right)\sum_{\alpha=1,2}\sum_{\epsilon\neq\epsilon'}\|G^{(\alpha)}_{\epsilon,\epsilon'}\|^2_{L^2(\Sigma_1\times\Sigma_1\times\Sigma_2)} < 1\ .$$

Then, for every g satisfying $|g| \le g_1$, H_W is a self-adjoint operator in $\mathfrak{F}$ with domain $\mathcal{D}(H_W) = \mathcal{D}(H_{W,0})$.

Ideas of the proof. The proof of this result is a trivial consequence of the following norm relative boundedness of $H_{W,I}$ with respect to $H_{W,0}$.

Lemma 2.3. *For any $\eta > 0$, $\beta > 0$, and $\psi \in \mathcal{D}(H_{W,0})$, we have*

$$
\begin{aligned}
&\|H_{W,I}\psi\| \\
&\le 6\sum_{\alpha=1,2}\sum_{\epsilon,\epsilon'}\|G^{(\alpha)}_{\epsilon,\epsilon'}\|^2\left(\frac{1}{2\mathrm{m}_W}\left(\frac{1}{\mathrm{m}_e{}^2}+1\right)+\frac{\beta}{2\mathrm{m}_W\mathrm{m}_e{}^2}+\frac{2\eta}{\mathrm{m}_e{}^2}(1+\beta)\right)\|H_{W,0}\psi\|^2 \\
&\quad+\left(\frac{1}{2\mathrm{m}_W}\left(1+\frac{1}{4\beta}\right)+2\eta\left(1+\frac{1}{4\beta}\right)+\frac{1}{2\eta}\right)\|\psi\|^2 .
\end{aligned}
\tag{2.7}
$$

Such a relative bound is obtained by using N_τ estimates of [21]. Details can be found in [13] and [4]. □

For the sequel, we shall make some of the following additional assumptions on the kernels $G^{(\alpha)}_{\epsilon,\epsilon'}$.

Hypothesis 2.4. *There exists* $\tilde{K}(G) < \infty$ *and* $\tilde{\tilde{K}}(G) < \infty$ *such that for* $\alpha = 1, 2,\ \epsilon, \epsilon' = \pm,\ i, j = 1, 2, 3,$ *and* $\sigma \geq 0$,

(i) $$\int_{\Sigma_1\times\Sigma_1\times\Sigma_2} \frac{|G^{(\alpha)}_{\epsilon,\epsilon'}(\xi_1,\xi_2,\xi_3)|^2}{|p_2|^2} \mathrm{d}\xi_1\mathrm{d}\xi_2\mathrm{d}\xi_3 < \infty\ ,$$

(ii) $$\left(\int_{\Sigma_1\times\left(\{|p_2|\leq\sigma\}\times\{-\frac{1}{2},\frac{1}{2}\}\right)\times\Sigma_2} |G^{(\alpha)}_{\epsilon,\epsilon'}(\xi_1,\xi_2,\xi_3)|^2 \mathrm{d}\xi_1\mathrm{d}\xi_2\mathrm{d}\xi_3\right)^{\frac{1}{2}} \leq \tilde{K}(G)\,\sigma\ ,$$

(iii-a) $(p_2\cdot\nabla_{p_2})G^{(\alpha)}_{\epsilon,\epsilon'}(.,.,.) \in L^2(\Sigma_1\times\Sigma_1\times\Sigma_2)$ *and*

$$\int_{\Sigma_1\times\left(\{|p_2|\leq\sigma\}\times\{-\frac{1}{2},\frac{1}{2}\}\right)\times\Sigma_2} \left|[(p_2\cdot\nabla_{p_2})G^{(\alpha)}_{\epsilon,\epsilon'}](\xi_1,\xi_2,\xi_3)\right|^2 \mathrm{d}\xi_1\mathrm{d}\xi_2\mathrm{d}\xi_3 < \tilde{\tilde{K}}(G)\,\sigma,$$

(iii-b) $$\int_{\Sigma_1\times\Sigma_1\times\Sigma_2} p_{2,i}^2\, p_{2,j}^2 \left|\frac{\partial^2 G^{(\alpha)}_{\epsilon,\epsilon'}}{\partial p_{2,i}\partial p_{2,j}}(\xi_1,\xi_2,\xi_3)\right|^2 \mathrm{d}\xi_1\mathrm{d}\xi_2\mathrm{d}\xi_3 < \infty\ .$$

Remark 2.5. Note that obviously, Hypothesis 2.4 (i) is stronger than Hypothesis 2.4 (ii).

Our first main result is the existence of a ground state for H_W together with the location of the spectrum of H_W.

Theorem 2.6 (Existence of a ground state and location of the spectrum). *Assume that the kernels* $G^{(\alpha)}_{\epsilon,\epsilon'}$ *satisfy Hypothesis* 2.1 *and* 2.4(i)*. Then, there exists* $g_2 \in (0, g_1]$ *such that* H_W *has a unique ground state for* $|g| < g_2$*. Moreover, for*

$$E = \inf \mathrm{Spec}(H_W)\,,$$

we have $E \leq 0$ *and the spectrum of* H_W *fulfills*

$$\mathrm{Spec}(H_W) = [E,\, \infty).$$

Ideas of the proof. The main ingredients of the proof of the existence of a ground state are the construction of infrared-cutoff operators and the existence of a gap above the ground state energy for these operators (see [13, Proposition 3.5]). This is an adaptation to our case of techniques due to Pizzo [40] and Bach, Fröhlich and Pizzo [5]. The details can be found in [13]. A different proof of the existence of a ground state can also be achieved by mimicking the proof given in [8].

The location of the spectrum follows from the existence of asymptotic Fock representations for the CAR associated with the neutrino creation and annihilation operators (see [34], [46] and [13]). □

Our next main result deals with the absolute continuity of the spectrum and local energy decay. Such a result is established using *standard Mourre theory*, and is a consequence of a limiting absorption principle. To state this result, we need to introduce the definition of the neutrino position operator B.

Let b be the operator in $L^2(\Sigma_1)$ accounting for the position of the neutrino

$$b = i\nabla_{p_2}\ , \quad \text{and let} \quad \langle b\rangle = (1+|b|^2)^{\frac{1}{2}}\ .$$

Its second quantized version $\mathrm{d}\Gamma(\langle b\rangle)$ is self-adjoint in $\mathfrak{F}_a(L^2(\Sigma_1))$. We thus define on $\mathfrak{F} = \mathfrak{F}_L \otimes \mathfrak{F}_W$ the position operator B for neutrinos and antineutrinos by

$$B = (\mathbb{1}\otimes\mathbb{1}\otimes \mathrm{d}\Gamma(\langle b\rangle)\otimes\mathbb{1})\otimes\mathbb{1}_{\mathfrak{F}_W} \ + \ (\mathbb{1}\otimes\mathbb{1}\otimes\mathbb{1}\otimes\mathrm{d}\Gamma(\langle b\rangle))\otimes\mathbb{1}_{\mathfrak{F}_W}\,.$$

We are now ready to state the main result concerning spectral and dynamical properties of H_W above the ground state energy. Note that the main achievement of Theorem 2.7 is to be able to prove absolute continuity of the spectrum and local energy decay down to the ground state energy *without* assuming any infrared regularization.

Theorem 2.7 (Absolutely continuous spectrum, Limiting Absorption Principle and Local Energy Decay). *Assume that the kernels $G^{(\alpha)}_{\epsilon,\epsilon'}$ satisfy Hypothesis* 2.1 *and* 2.4(ii)–(iii). *For any $\delta > 0$ satisfying $0 < \delta < \mathrm{m}_e$, there exists $g_\delta > 0$ such that for $0 < |g| < g_\delta$:*

(i) *The spectrum of H_W in $(E,\, E+\mathrm{m}_e-\delta]$ is purely absolutely continuous.*
(ii) *For $s > 1/2$, $\varphi\in\mathfrak{F}$, and $\psi\in\mathfrak{F}$, the limits*

$$\lim_{\epsilon\to 0}(\varphi,\, \langle B\rangle^{-s}(H_W-\lambda\pm i\epsilon)\langle B\rangle^{-s}\psi)$$

exist uniformly for λ in every compact subset of $(E,\, E+\mathrm{m}_e-\delta)$.
(iii) *For $s\in(1/2,\,1)$ and $f\in C_0^\infty((E,\, E+\mathrm{m}_e-\delta))$, we have*

$$\big\|(B+1)^{-s}\mathrm{e}^{-itH_W}f(H_W)(B+1)^{-s}\big\| = \mathcal{O}\big(t^{-(s-1/2)}\big)\,.$$

Ideas of the proof. The main problem we face is that the bottom of the spectrum E is a threshold of the total Hamiltonian H_W by our choice of the conjugate operator. This renders the analysis of the spectrum and of the dynamics close to E difficult. To overcome this difficulty, it is not possible to adapt the proof of Fröhlich, Griesemer and Sigal [19] used in the context of nonrelativistic QED, since in [19] it is possible to regularize the infrared behavior of the interaction by using a unitary Pauli–Fierz transformation that has no equivalent for our model. Instead, to circumvent infrared difficulties, and to avoid infrared regularization of [13], we adapt to our context the proof of [14] established for a model of non-relativistic QED for a free electron at fixed total momentum. Due to the complicated structure of their interaction operator, the authors in [14] used some Feshbach–Schur map before proving a Mourre estimate for an effective Hamiltonian. Here, thanks to some specific estimates that we can derive for our model, we do not need to apply such a map, and we obtain a Mourre estimate directly for H_W.

The main steps of the proof are as follows (details can be found in [4]):

The regularity assumptions Hypothesis 2.4(iii-a) and (iii-b) on the kernels allow us to establish a Mourre estimate (Theorem 2.8) and a limiting absorption principle (Theorem 2.10) for any spectral interval down to the energy of the ground state and below the mass of the electron. Hence, the whole spectrum between the ground state and the first threshold is purely absolutely continuous.

To prove Theorems 2.10 and 2.8, we first approximate the total Hamiltonian H_W by a cutoff Hamiltonian $H_{W,\sigma}$ with the property that the interaction between the massive particles and the neutrinos or antineutrinos of energies $\leq \sigma$ has been suppressed. We denote by H_W^σ the restriction of $H_{W,\sigma}$ to the Fock space for the massive particles together with the neutrinos and antineutrinos of energies $\geq \sigma$. Then, as in [13], adapting the method of [5], we prove that for some suitable sequence $\sigma_n \to 0$, the Hamiltonian $H_W^{\sigma_n}$ has a gap of size $\sim \sigma_n$ in its spectrum above its ground state energy for all $n \in \mathbb{N}$.

Thus, we use this gap property in combination with the conjugate operator method developed in [3] and [44] in order to establish a Mourre estimate for a sequence of energy intervals $(\Delta_n)_{n\geq 0}$ smaller and smaller, accumulating at the ground state energy of H_W, and covering the interval $(E,\, E + \mathrm{m}_e - \delta)$. This requires to build up a sequence $(A_n^{(\tau)})_{n\geq 0}$ of generators that only affects the massless particles of low energies. For each n, the *self-adjoint conjugate operators* $A_n^{(\tau)}$ is the generator of dilatations in the Fock space for neutrinos and antineutrinos *with a cutoff in the momentum variable*, and is defined as follows.

Set $\tau := 1 - \delta/(2(2\mathrm{m}_e - \delta))$, $\gamma := 1 - \delta/(2\mathrm{m}_e - \delta)$ and define $\chi^{(\tau)} \in C^\infty(\mathbb{R},\, [0,1])$ as

$$\chi^{(\tau)}(\lambda) = \begin{cases} 1 & \text{for } \lambda \in (-\infty,\, \tau]\,, \\ 0 & \text{for } \lambda \in [1,\, \infty)\,. \end{cases}$$

For the sequence of small neutrino momentum cutoffs $(\sigma_n)_{n\geq 0}$ given by $\sigma_0 = 2\mathrm{m}_e + 1$, $\sigma_1 = \mathrm{m}_e - \delta/2$ and for $n \geq 1$, $\sigma_{n+1} = \gamma\sigma_n$, we define, for all $p_2 \in \mathbb{R}^3$ and $n \geq 1$,

$$\chi_n^{(\tau)}(p_2) = \chi^{(\tau)}\left(\frac{|p_2|}{\sigma_n}\right).$$

The one-particle (neutrino) conjugate operator is

$$a_n^{(\tau)} = \chi_n^{(\tau)}(p_2)\frac{1}{2}\left(p_2 \cdot i\nabla_{p_2} + i\nabla_{p_2} \cdot p_2\right)\chi_n^{(\tau)}(p_2),$$

and its second quantized version is

$$A_n^{(\tau)} = \mathbb{1} \otimes \mathrm{d}\Gamma(a_n^{(\tau)}) \otimes \mathbb{1}, \tag{2.8}$$

where, as above, $\mathrm{d}\Gamma(\cdot)$ refers to the usual second quantization of one particle operators. We also set

$$\langle A_n^{(\tau)} \rangle = (1 + (A_n^{(\tau)})^2)^{\frac{1}{2}}\,.$$

The operators $a_n^{(\tau)}$ and $A_n^{(\tau)}$ are self-adjoint.

Let $(\Delta_n)_{n\geq 0}$ be a sequence of open sets covering any compact subset of $(\inf \mathrm{Spec}(H_W),\, \mathrm{m}_e - \delta)$ be defined as $\Delta_n := [(\gamma - \epsilon_\gamma)^2\sigma_n,\, (\gamma + \epsilon_\gamma)\sigma_n]$, where $\epsilon_\gamma > 0$ is fixed and small enough.

Using the spectral gap result for H^{σ_n}, relative bounds as in Lemma 2.3 and Helffer–Sjöstrand calculus (see details in [4, § 5]), we obtain

Theorem 2.8 (Mourre inequality). *Suppose that the kernels $G^{(\alpha)}_{\epsilon,\epsilon'}$ satisfy Hypothesis* 2.1, 2.4(ii), *and* 2.4(iii.a). *Then, there exists $C_\delta > 0$ and $g_\delta > 0$ such that, for $|g| < g_\delta$ and $n \geq 1$,*

$$E_{\Delta_n}(H_W - E)\,[H_W,\, iA_n^{(\tau)}]\,E_{\Delta_n}(H_W - E) \geq C_\delta \frac{\gamma^2}{N^2}\,\sigma_n\,E_{\Delta_n}(H_W - E)\,. \qquad (2.9)$$

Then we establish a regularity result of H_W with respect to the conjugate operator $A_n^{(\tau)}$.

Theorem 2.9 ($C^2(A_n^{(\tau)})$-regularity). *Suppose that the kernels $G^{(\alpha)}_{\epsilon,\epsilon'}$ satisfy Hypothesis* 2.1 *and Hypothesis* 2.4(iii). *Then, H_W is locally of class $C^2(A_n^{(\tau)})$ in $(-\infty, \mathrm{m}_e - \delta/2)$ for every $n \geq 1$.*

The proof of this result is a straightforward adaptation of [13, Theorem 3.7], substituting there A by $A_n^{(\tau)}$.

Now, according to Theorems 0.1 and 0.2 in [44] (see also [28], [25], and [19]), the $C^2(A_n^{(\tau)})$-regularity in Theorem 2.9 and the Mourre inequality in Theorem 2.8 imply the following limiting absorption principle for sufficiently small coupling constants.

Theorem 2.10 (Limiting absorption principle). *Suppose that the kernels $G^{(\alpha)}_{\epsilon,\epsilon'}$ satisfy Hypothesis* 2.1, 2.4(ii), 2.4(iii). *Then, for any $\delta > 0$ satisfying $0 < \delta < \mathrm{m}_e/2$, there exists $g_\delta > 0$ such that, for $|g| < g_\delta$, for $s > 1/2$, φ, $\psi \in \mathfrak{F}$ and for $n \geq 1$, the limits*

$$\lim_{\epsilon \to 0}(\varphi,\, \langle A_n^{(\tau)}\rangle^{-s}(H_W - \lambda \pm i\epsilon)\langle A_n^{(\tau)}\rangle^{-s}\psi)$$

exist uniformly for $\lambda \in \Delta_n$. Moreover, for $1/2 < s < 1$, the map

$$\lambda \mapsto \langle A_n^{(\tau)}\rangle^{-s}(H_W - \lambda \pm i0)^{-1}\langle A_n^{(\tau)}\rangle^{-s}$$

is Hölder continuous of order $s - 1/2$ in Δ_n.

Eventually, the proof of Theorem 2.7 is a direct consequence of the limiting absorption principle. The absolutely continuous spectrum is deduced from [44, Theorem 0.1 and Theorem 0.2], and the dynamical properties are derived in the usual way. □

3. Interaction of the gauge boson Z^0 with an electron and a positron

In this section, we do the spectral analysis for the Hamiltonian associated to the decay of the vector boson Z^0 into electrons and positrons,

$$Z^0 \to e^- + e^+ .$$

The interaction between the electrons/positrons and the vector bosons Z^0, in the Schrödinger representation is given, up to a coupling constant, by (see [30, (4.139)] and [50, (21.3.20)])

$$I_{Z^0} = \int \overline{\Psi_e}(x)\gamma^\alpha(g'_V - \gamma_5)\Psi_e(x)Z_\alpha(x)\,\mathrm{d}x + h.c., \tag{3.1}$$

where γ^α, $\alpha = 0,1,2,3$, and γ_5 are the Dirac matrices, g'_V is a real parameter such that $g'_V \simeq 0,074$ (see, e.g., [30]), $\Psi_e(x)$ and $\overline{\Psi_e}(x)$ are the Dirac fields for the electron e_- and the positron e_+ of mass m_e, and Z_α is the massive boson field for Z^0.

The field $\Psi_e(x)$ is formally defined by

$$\Psi_e(x) = \int \psi_+(\xi,\, x)b_+(\xi) + \widetilde{\psi}_-(\xi,\, x)b^*_-(\xi)\,\mathrm{d}\xi,$$

with

$$\widetilde{\psi}_-(\xi,\, x) = \widetilde{\psi}_-((p,\gamma),\, x) = \psi_-((p,(j,-m_j,-\kappa_j)),x) \tag{3.2}$$

and where $\psi_\pm(\xi,\, x)$ are the generalized eigenfunctions associated with the continuous spectrum of the free Dirac operator labeled by the total angular momentum quantum numbers j and m_j, and the quantum numbers κ_j.

The boson field Z_α is formally defined by (see, e.g., [49, Eq. (5.3.34)]),

$$Z_\alpha(x) = (2\pi)^{-\frac{3}{2}} \int \frac{\mathrm{d}\xi_3}{(2(|k|^2+\mathrm{m}_{Z^0}{}^2)^{\frac{1}{2}})^{\frac{1}{2}}} \Big(\epsilon_\alpha(k,\lambda)a(\xi_3)\mathrm{e}^{ik.x} + \epsilon^*_\alpha(k,\lambda)a^*(\xi_3)\mathrm{e}^{-ik.x}\Big),$$

where the vectors $\epsilon_\alpha(k,\lambda)$ are the polarizations vectors of the massive spin 1 bosons (see [49, Section 5.3]), and with $\xi_3 = (k,\,\lambda)$, where $k \in \mathbb{R}^3$ is the momentum variable of the boson and $\lambda \in \{-1,0,1\}$ is its polarization.

If one considers, as mentioned in the introduction, the full interaction I_{Z^0} in (3.1) describing the decay of the gauge boson Z^0 into massive leptons and if one formally expands this interaction with respect to products of creation and annihilation operators, we are left with a finite sum of terms with kernels yielding singular operators which cannot be defined as closed operators. Therefore, in order to obtain a well-defined Hamiltonian (see, e.g., [21, 7, 8, 13, 4]), we replace these kernels by square integrable functions $G^{(\alpha)}$. In particular, this implies large momentum cutoffs for the electrons, positrons and Z^0 bosons. Moreover, we confine in space the interaction between the electrons/positrons and the bosons by adding a localization function $f(|x|)$, with $f \in \mathrm{C}_0^\infty([0,\infty))$.

3.1. Rigorous definition of the model

3.1.1. The Fock spaces for electrons, positrons and Z^0 bosons. In order to properly define the interaction I_{Z^0} formally introduced above, since we use a spectral representation of the free Dirac operator generated by the sequence of spherical waves, we first recall a few facts about solutions of the free Dirac equation.

The energy of a free relativistic electron of mass m_e is described by the self-adjoint Dirac Hamiltonian

$$H_D = \boldsymbol{\alpha} \cdot (1/i)\nabla + \boldsymbol{\beta}\, \mathrm{m}_e,$$

(see [42, 47] and references therein) acting on the Hilbert space $\mathfrak{H} = L^2(\mathbb{R}^3; \mathbb{C}^4)$, with domain $\mathfrak{D}(H_D) = H^1(\mathbb{R}^3; \mathbb{C}^4)$. We use the system of units $\hbar = c = 1$. Here $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and $\boldsymbol{\beta}$ are the Dirac matrices in the standard form.

The generalized eigenfunctions associated with the continuous spectrum of the Dirac operator H_D are labeled by the total angular momentum quantum numbers

$$j \in \left\{ \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots \right\}, \qquad m_j \in \{-j, -j+1, \dots, j-1, j\}, \tag{3.3}$$

and by the quantum numbers

$$\kappa_j \in \left\{ \pm \left(j + \frac{1}{2} \right) \right\}. \tag{3.4}$$

In the sequel, we will drop the index j and set

$$\gamma = (j,\, m_j,\, \kappa_j)\,, \tag{3.5}$$

and a sum over γ will thus denote a sum over j, m_j and κ_j. We denote by Γ the set $\{(j,\, m_j,\, \kappa_j),\ j \in \mathbb{N} + \frac{1}{2},\ m_j \in \{-j, -j+1, \dots, j-1, j\},\ \kappa_j \in \{\pm(j + \frac{1}{2})\}\}$.

For $\mathbf{p} \in \mathbb{R}^3$ being the momentum of the electron, and $p := |\mathbf{p}|$, the continuum energy levels are given by $\pm\,\omega(p)$, where

$$\omega(p) := ({\mathrm{m}_e}^2 + p^2)^{\frac{1}{2}}\,. \tag{3.6}$$

We introduce the notation

$$\xi = (p,\, \gamma)\ \in \mathbb{R}_+ \times \Gamma. \tag{3.7}$$

The continuum eigenstates of H_D are denoted by

$$\psi_\pm(\xi, x) = \psi_\pm((p, \gamma), x)\,.$$

We then have

$$H_D\ \psi_\pm((p,\gamma),x) = \pm\,\omega(p)\ \psi_\pm((p,\gamma),x).$$

The generalized eigenstates $\psi_\pm$ are normalized in such a way that

$$\int_{\mathbb{R}^3} \psi_\pm^\dagger((p,\gamma),x)\, \psi_\pm((p',\gamma'),x)\, \mathrm{d}x = \delta_{\gamma\gamma'}\delta(p-p'),$$

$$\int_{\mathbb{R}^3} \psi_\pm^\dagger((p,\gamma),x)\, \psi_\mp((p',\gamma'),x)\, \mathrm{d}x = 0\,.$$

Here $\psi_\pm^\dagger((p,\gamma),\, x)$ is the adjoint spinor of $\psi_\pm((p,\gamma),\, x)$.

According to the hole theory [42, 43, 47, 49], the absence in the Dirac theory of an electron with energy $E < 0$ and charge e is equivalent to the presence of a positron with energy $-E > 0$ and charge $-e$.

Let us split the Hilbert space $\mathfrak{H} = L^2(\mathbb{R}^3; \mathbb{C}^4)$ into

$$\mathfrak{H}_{c^-} = P_{(-\infty, -\mathrm{m}_e]}(H_D)\mathfrak{H} \quad \text{and} \quad \mathfrak{H}_{c^+} = P_{[\mathrm{m}_e, +\infty)}(H_D)\mathfrak{H}.$$

Here $P_I(H_D)$ denotes the spectral projection of H_D corresponding to the interval I.

Let $\Sigma := \mathbb{R}_+ \times \Gamma$. We can identify the Hilbert spaces $\mathfrak{H}_{c^\pm}$ with

$$\mathfrak{H}_c := L^2(\Sigma; \mathbb{C}^4) \simeq \oplus_\gamma L^2(\mathbb{R}_+; \mathbb{C}^4)\,,$$

by using the unitary operators $U_{c^\pm}$ defined from $\mathfrak{H}_{c^\pm}$ to $\mathfrak{H}_c$ via the identities in the L^2 sense

$$(U_{c^\pm}\phi)(p, \gamma) = \int \psi_\pm^\dagger((p, \gamma)\,, x)\,\phi(x)\,\mathrm{d}x\,. \tag{3.8}$$

On $\mathfrak{H}_c$, we define the scalar products

$$(g,\, h) = \int \overline{g(\xi)} h(\xi) \mathrm{d}\xi = \sum_{\gamma \in \Gamma} \int_{\mathbb{R}^+} \overline{g(p, \gamma)} h(p, \gamma)\,\mathrm{d}p\,. \tag{3.9}$$

In the sequel, we shall denote the variable $(p,\, \gamma)$ by $\xi_1 = (p_1, \gamma_1)$ in the case of electrons, and $\xi_2 = (p_2, \gamma_2)$ in the case of positrons, respectively.

We next introduce the Fock space for electrons and positrons.

Let

$$\mathfrak{F}_a := \mathfrak{F}_a(\mathfrak{H}_c) = \bigoplus_{n=0}^{\infty} \otimes_a^n \mathfrak{H}_c,$$

be the Fermi–Fock space over $\mathfrak{H}_c$, and let

$$\mathfrak{F}_D := \mathfrak{F}_a \otimes \mathfrak{F}_a$$

be the Fermi–Fock space for electrons and positrons, with vacuum Ω_D.

The creation and annihilation operators for electrons and positrons are defined as follows.

We set, for every $g \in \mathfrak{H}_c$,

$$b_{\gamma,+}(g) = b_+(P_\gamma g)\,, \quad b_{\gamma,+}^*(g) = b_+^*(P_\gamma g)\,,$$

where P_γ is the projection of $\mathfrak{H}_c$ onto the γth component defined according to (3.8), and $b_+(P_\gamma g)$ and $b_+^*(P_\gamma g)$ are respectively the annihilation and creation operator for an electron.

As above, we set, for every $h \in \mathfrak{H}_c$,

$$b_{\gamma,-}(h) = b_-(P_\gamma h)\,,$$
$$b_{\gamma,-}^*(h) = b_-^*(P_\gamma h)\,,$$

where $b_-(P_\gamma g)$ and $b_-^*(P_\gamma g)$ are respectively the annihilation and creation operator for a positron.

As in [41, Chapter X], we introduce operator-valued distributions $b_\pm(\xi)$ and $b^*_\pm(\xi)$ that fulfill for $g \in \mathfrak{H}_c$,

$$b_\pm(g) = \int b_\pm(\xi)\, \overline{(P_\gamma g)\,(p)}\, \mathrm{d}\xi$$

$$b^*_\pm(g) = \int b^*_{\gamma,\pm}(p)\,(P_\gamma g)\,(p)\, \mathrm{d}\xi$$

where we used the notation of (3.9).

We give here the construction of the Fock space for the Z^0 boson.

Let

$$\Sigma_3 := \mathbb{R}^3 \times \{-1,\, 0,\, 1\}\,.$$

The one-particle Hilbert space for the particle Z^0 is $L^2(\Sigma_3)$ with scalar product

$$(f,\, g) = \int_{\Sigma_3} \overline{f(\xi_3)} g(\xi_3) \mathrm{d}\xi_3\,, \tag{3.10}$$

with the notations

$$\xi_3 = (k,\, \lambda) \quad \text{and} \quad \int_{\Sigma_3} \mathrm{d}\xi_3 = \sum_{\lambda=-1,0,1} \int_{\mathbb{R}^3} \mathrm{d}k\,, \tag{3.11}$$

where $\xi_3 = (k,\, \lambda) \in \Sigma_3$.

The bosonic Fock space for the vector boson Z^0, denoted by $\mathfrak{F}_{Z^0}$, is thus the symmetric Fock space

$$\mathfrak{F}_{Z^0} = \mathfrak{F}_s(L^2(\Sigma_3))\,. \tag{3.12}$$

For $f \in L^2(\Sigma_3)$, we define the annihilation and creation operators, denoted by $a(f)$ and $a^*(f)$ by

$$a(f) = \int_{\Sigma_3} \overline{f(\xi_3)} a(\xi_3) \mathrm{d}\xi_3 \tag{3.13}$$

and

$$a^*(f) = \int_{\Sigma_3} f(\xi_3) a^*(\xi_3) \mathrm{d}\xi_3 \tag{3.14}$$

where the operators $a(\xi_3)$ (respectively $a^*(\xi_3)$) are the bosonic annihilation (respectively bosonic creation) operator for the boson Z^0 (see, e.g., [36, 12, 13]).

3.1.2. The Hamiltonian. The quantization of the Dirac Hamiltonian H_D, acting on $\mathfrak{F}_D$, is given by

$$T_D = \int \omega(p)\, b^*_+(\xi_1)\, b_+(\xi_1) \mathrm{d}\xi_1 \;+\; \int \omega(p)\, b^*_-(\xi_2)\, b_-(\xi_2) \mathrm{d}\xi_2,$$

with $\omega(p)$ given in (3.6). The operator T_D is the Hamiltonian of the quantized Dirac field.

Let $\mathfrak{D}_D$ denote the set of vectors $\Phi \in \mathfrak{F}_D$ for which $\Phi^{(r,s)}$ is smooth and has a compact support and $\Phi^{(r,s)} = 0$ for all but finitely many (r, s). Then T_D is well defined on the dense subset $\mathfrak{D}_D$ and it is essentially self-adjoint on $\mathfrak{D}_D$.

The self-adjoint extension will be denoted by the same symbol T_D, with domain $\mathfrak{D}(T_D)$.

The operators number of electrons and number of positrons, denoted respectively by N_+ and N_-, are given by

$$N_+ = \int b_+^*(\xi_1)\, b_+(\xi_1) \mathrm{d}\xi_1 \quad \text{and} \quad N_- = \int b_-^*(\xi_2)\, b_-(\xi_2) \mathrm{d}\xi_2 \,. \tag{3.15}$$

They are essentially self-adjoint on $\mathfrak{D}_D$.

We have

$$\mathrm{Spec}(T_D) = \{0\} \cup [\mathrm{m}_e, \infty).$$

The set $[\mathrm{m}_e, \infty)$ is the absolutely continuous spectrum of T_D.

The Hamiltonian of the bosonic field, acting on $\mathfrak{F}_{Z^0}$, is

$$T_Z := \int \omega_3(k)\, a^*(\xi_3) a(\xi_3)\, \mathrm{d}\xi_3$$

where

$$\omega_3(k) = \sqrt{|k|^2 + {\mathrm{m}_{Z^0}}^2}. \tag{3.16}$$

The operator T_Z is essentially self-adjoint on the set of vectors $\Phi \in \mathfrak{F}_{Z^0}$ such that $\Phi^{(n)}$ is smooth and has compact support and $\Phi^{(n)} = 0$ for all but finitely many n. Its self-adjoint extension is denoted by the same symbol.

The spectrum of T_Z consists of an absolutely continuous spectrum covering $[\mathrm{m}_{Z^0}, \infty)$ and a simple eigenvalue, equal to zero, whose corresponding eigenvector is the vacuum state $\Omega_s \in \mathfrak{F}_{Z^0}$.

The free Hamiltonian is defined on $\mathcal{H} := \mathfrak{F}_D \otimes \mathfrak{F}_{Z^0}$ by

$$H_{Z,0} = T_D \otimes \mathbb{1} + \mathbb{1} \otimes T_Z \,. \tag{3.17}$$

The operator $H_{Z,0}$ is essentially self-adjoint on $\mathfrak{D}(T_D) \otimes \mathfrak{D}(T_Z)$. Since $\mathrm{m}_e < \mathrm{m}_{Z^0}$, the spectrum of $H_{Z,0}$ is given by

$$\mathrm{Spec}(H_{Z,0}) = \{0\} \cup [\mathrm{m}_e,\, \infty) \,.$$

More precisely,

$$\mathrm{Spec}_{\mathrm{pp}}(H_{Z,0}) = \{0\}, \quad \mathrm{Spec}_{\mathrm{sc}}(H_{Z,0}) = \emptyset, \quad \mathrm{Spec}_{\mathrm{ac}}(H_{Z,0}) = [\mathrm{m}_e,\, \infty), \tag{3.18}$$

where $\mathrm{Spec}_{\mathrm{pp}}$, $\mathrm{Spec}_{\mathrm{sc}}$, $\mathrm{Spec}_{\mathrm{ac}}$ denote the pure point, singular continuous and absolutely continuous spectra, respectively. Furthermore, 0 is a non-degenerate eigenvalue associated to the vacuum $\Omega_D \otimes \Omega_s$.

The interaction Hamiltonian is defined on $\mathcal{H} = \mathfrak{F}_D \otimes \mathfrak{F}_{Z^0}$ by

$$H_{Z,I} = H_{Z,I}^{(1)} + {H_{Z,I}^{(1)}}^* + H_{Z,I}^{(2)} + {H_{Z,I}^{(2)}}^* \,, \tag{3.19}$$

with

$$\begin{aligned}
H_{Z,I}^{(1)} = & \int \left(\int_{\mathbb{R}^3} f(|x|) \overline{\psi_+(\xi_1,\, x)} \gamma^\mu (g_V' - \gamma_5) \widetilde{\psi}_-(\xi_2,\, x) \frac{\epsilon_\mu(\xi_3)}{\sqrt{2\omega_3(k)}} \, \mathrm{e}^{ik\cdot x} \, \mathrm{d}x \right) \qquad (3.20) \\
& \times G^{(1)}(\xi_1,\, \xi_2,\, \xi_3) b_+^*(\xi_1) b_-^*(\xi_2) a(\xi_3) \, \mathrm{d}\xi_1 \mathrm{d}\xi_2 \mathrm{d}\xi_3 \,, \\
H_{Z,I}^{(1)\,*} = & \int \left(\int_{\mathbb{R}^3} f(|x|) \overline{\widetilde{\psi}_-(\xi_2,\, x)} \gamma^\mu (g_V' - \gamma_5) \psi_+(\xi_1,\, x) \frac{\epsilon_\mu^*(\xi_3)}{\sqrt{2\omega_3(k)}} \, \mathrm{e}^{-ik\cdot x} \, \mathrm{d}x \right) \qquad (3.21) \\
& \times \overline{G^{(1)}(\xi_1,\, \xi_2,\, \xi_3)} a^*(\xi_3) b_-(\xi_2) b_+(\xi_1) \, \mathrm{d}\xi_1 \mathrm{d}\xi_2 \mathrm{d}\xi_3 \,, \\
H_{Z,I}^{(2)} = & \int \left(\int_{\mathbb{R}^3} f(|x|) \overline{\psi_+(\xi_1,\, x)} \gamma^\mu (g_V' - \gamma_5) \widetilde{\psi}_-(\xi_2,\, x) \frac{\epsilon_\mu^*(\xi_3)}{\sqrt{2\omega_3(k)}} \, \mathrm{e}^{-ik\cdot x} \, \mathrm{d}x \right) \qquad (3.22) \\
& \times G^{(2)}(\xi_1,\, \xi_2,\, \xi_3) b_+^*(\xi_1) b_-^*(\xi_2) a^*(\xi_3) \, \mathrm{d}\xi_1 \mathrm{d}\xi_2 \mathrm{d}\xi_3 \,,
\end{aligned}$$

and

$$\begin{aligned}
H_{Z,I}^{(2)\,*} = & \int \left(\int_{\mathbb{R}^3} f(|x|) \overline{\widetilde{\psi}_-(\xi_2,\, x)} \gamma^\mu (g_V' - \gamma_5) \psi_+(\xi_1,\, x) \frac{\epsilon_\mu(\xi_3)}{\sqrt{2\omega_3(k)}} \, \mathrm{e}^{ik\cdot x} \, \mathrm{d}x \right) \qquad (3.23) \\
& \times \overline{G^{(2)}(\xi_1,\, \xi_2,\, \xi_3)} a(\xi_3) b_-(\xi_2) b_+(\xi_1) \, \mathrm{d}\xi_1 \mathrm{d}\xi_2 \mathrm{d}\xi_3 \,.
\end{aligned}$$

Performing the integration with respect to x in the expressions above, we see that $H_{Z,I}^{(1)}$ and $H_{Z,I}^{(2)}$ can be written in the form

$$\begin{aligned}
H_{Z,I}^{(1)} &:= H_{Z,I}^{(1)}(F^{(1)}) := \int F^{(1)}(\xi_1,\, \xi_2,\, \xi_3) b_+^*(\xi_1) b_-^*(\xi_2) a(\xi_3) \, \mathrm{d}\xi_1 \mathrm{d}\xi_2 \mathrm{d}\xi_3 \,, \\
H_{Z,I}^{(2)} &:= H_{Z,I}^{(2)}(F^{(2)}) := \int F^{(2)}(\xi_1,\, \xi_2,\, \xi_3) b_+^*(\xi_1) b_-^*(\xi_2) a^*(\xi_3) \, \mathrm{d}\xi_1 \mathrm{d}\xi_2 \mathrm{d}\xi_3 \,,
\end{aligned} \qquad (3.24)$$

where, for $\alpha = 1, 2$,

$$F^{(\alpha)}(\xi_1,\, \xi_2,\, \xi_3) := h^{(\alpha)}(\xi_1, \xi_2, \xi_3) G^{(\alpha)}(\xi_1, \xi_2, \xi_3), \qquad (3.25)$$

and $h^{(1)}(\xi_1, \xi_2, \xi_3)$, $h^{(2)}(\xi_1, \xi_2, \xi_3)$ are given by the integral over x in (3.20) and (3.22), respectively.

Our main result, Theorem 3.5 below, requires the functions $F^{(\alpha)}$ to be sufficiently regular near $p_1 = 0$ and $p_2 = 0$ (where, recall, $\xi_l = (p_l, \gamma_l)$ for $l = 1, 2$).

Note that this regularity is required for applying the conjugate operator method. In practice, starting from the physical (ill-defined) Hamiltonian, applying UV cutoffs $G_{\epsilon,\epsilon'}^{(\alpha)}$ and a space localization $f(|x|)$ to the interaction $H_{Z,I}$ as done above, this regularity is fulfilled, except, solely, for the part of the field corresponding to quantum number $j = 1/2$. This is a consequence of a careful analysis of the behavior for momenta p close to zero of the generalized eigenstates $\psi_+(\xi,\, x) = \psi_+((p, (j, m_j, \kappa_j); x)$ and their derivatives have a too singular behavior at $\xi = 0$. This analysis is done in [9, Appendix A]).

The total Hamiltonian of the decay of the boson Z^0 into an electron and a positron is

$$H_Z := H_{Z,0} + g\, H_{Z,I},$$

where g is a real coupling constant.

3.2. Limiting absorbtion principle and spectral properties

For $p \in \mathbb{R}_+$, $j \in \{\frac{1}{2}, \frac{3}{2}, \dots\}$, $\gamma = (j,\, m_j,\, \kappa_j)$ and $\gamma_j = j + \frac{1}{2}$, we define

$$A(\xi) = A(p,\gamma) := \frac{(2p)^{\gamma_j+1}}{\Gamma(\gamma_j)} \left(\frac{\omega(p)+\mathrm{m}_e}{\omega(p)}\right)^{\frac{1}{2}} \left(\int_0^\infty |f(r)| r^{2\gamma_j}(1+r^2)\mathrm{d}r\right)^{\frac{1}{2}}, \quad (3.26)$$

where Γ denotes Euler's Gamma function, and $f \in \mathrm{C}_0^\infty([0,\infty))$ is the localization function appearing in (3.20)–(3.23). We make the following hypothesis on the kernels $G^{(\alpha)}$.

Hypothesis 3.1. *For* $\alpha = 1, 2$,

$$\int A(\xi_1)^2 A(\xi_2)^2 (|k|^2 + {\mathrm{m}_{Z^0}}^2)^{\frac{1}{2}} \left|G^{(\alpha)}(\xi_1,\, \xi_2,\, \xi_3)\right|^2 \mathrm{d}\xi_1 \mathrm{d}\xi_2 \mathrm{d}\xi_3 < \infty. \quad (3.27)$$

Note that up to universal constants, the functions $A(\xi)$ in (3.26) are upper bounds for the integrals with respect to x that occur in (3.20). These bounds are derived using the inequality (see [49, Eq. (5.3.23)–(5.3.25)])

$$\left|\frac{\epsilon_\mu(\xi_3)}{\sqrt{2\omega_3(k)}}\right| \le C_{\mathrm{m}_{Z^0}} (1 + |k|^2)^{\frac{1}{4}}\,. \quad (3.28)$$

For $C_Z := 156\, C_{\mathrm{m}_{Z^0}}$, let us define

$$K_1(G^{(\alpha)})^2 := {C_Z}^2 \left(\int A(\xi_1)^2 A(\xi_2)^2\, |G^{(\alpha)}(\xi_1,\, \xi_2,\, \xi_3)|^2 \mathrm{d}\xi_1 \mathrm{d}\xi_2 \mathrm{d}\xi_3\right), \quad (3.29)$$

$$K_2(G^{(\alpha)})^2 := {C_Z}^2 \left(\int A(\xi_1)^2 A(\xi_2)^2\, |G^{(\alpha)}(\xi_1,\, \xi_2,\, \xi_3)|^2 (|k|^2+1)^{\frac{1}{2}} \mathrm{d}\xi_1 \mathrm{d}\xi_2 \mathrm{d}\xi_3\right).$$

Our fist result is a basic result on self-adjointness.

Theorem 3.2 (Self-adjointness). *Assume that Hypothesis* 3.1 *holds. Let* $g_0 > 0$ *be such that*

$$ {g_0}^2 \left(\sum_{\alpha=1,2} K_1(G^{(\alpha)})^2\right) \left(\frac{1}{{\mathrm{m}_e}^2} + 1\right) < 1\,. \quad (3.30)$$

Then for any real g *such that* $|g| \le g_0$*, the operator* $H_Z = H_{Z,0} + gH_{Z,I}$ *is self-adjoint with domain* $\mathfrak{D}(H_{Z,0})$*. Moreover, any core for* $H_{Z,0}$ *is a core for* H_Z*.*

Notice that combining (3.18), relative boundedness of $H_{Z,I}$ with respect to $H_{Z,0}$ and standard perturbation theory of isolated eigenvalues (see, e.g., [37]), we deduce that, for $|g| \ll \mathrm{m}_e$, $\inf \mathrm{Spec}(H_Z)$ is a non-degenerate eigenvalue of H_Z. In other words, H_Z admits a unique ground state.

Theorem 3.2 follows from the Kato–Rellich Theorem together with standard estimates of creation and annihilation operators in Fock space, showing that the interaction Hamiltonian $H_{Z,I}$ is relatively bounded with respect to $H_{Z,0}$.

To establish our next theorems, we need to strengthen the conditions on the kernels $G^{(\alpha)}$.

Hypothesis 3.3. *For $\alpha = 1, 2$, the kernels $G^{(\alpha)} \in L^2(\Sigma \times \Sigma \times \Sigma_3)$ satisfy*

(i) *There exists a compact set $K \subset \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{R}^3$ such that*

$$G^{(\alpha)}(p_1, \gamma_1, p_2, \gamma_2, k, \lambda) = 0$$

if $(p_1, p_2, k) \notin K$.

(ii) *There exists $\varepsilon \geq 0$ such that*

$$\sum_{\gamma_1,\gamma_2,\lambda} \int (1 + x_1^2 + x_2^2)^{1+\varepsilon} \left| \hat{G}^{(\alpha)}(x_1, \gamma_1, x_2, \gamma_2, k, \lambda) \right|^2 \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}k < \infty,$$

where $\hat{G}^{(\alpha)}$ denotes the Fourier transform of $G^{(\alpha)}$ with respect to the variables (p_1, p_2), and x_j is the variable dual to p_j.

(iii) *If $\gamma_{1j} = 1$ or $\gamma_{2j} = 1$, where for $l = 1, 2$, $\gamma_{lj} = |\kappa_{j_l}|$ (with $\gamma_l = (j_l, m_{j_l}, \kappa_{j_l})$), and if $p_1 = 0$ or $p_2 = 0$, then $G^{(\alpha)}(p_1, \gamma_1, p_2, \gamma_2, k, \lambda) = 0$.*

Remark.

1) The assumption that $G^{(\alpha)}$ is compactly supported in the variables (p_1, p_2, k) is an "ultraviolet" constraint that is made for convenience. It could be replaced by the weaker assumption that $G^{(\alpha)}$ decays sufficiently fast at infinity.
2) Hypothesis 3.3(ii) comes from the fact that the coupling functions $G^{(\alpha)}$ must satisfy some "minimal" regularity for our method to be applied. In fact, Hypothesis (ii) could be slightly improved with a refined choice of interpolation spaces in our proof. In Hypothesis 3.3(iii), we need in addition an "infrared" regularization. We remark in particular that Hypotheses (ii) and (iii) imply that, for $0 \leq \varepsilon < 1/2$,

$$\left| G^{(\alpha)}(p_1, \gamma_1, p_2, \gamma_2, k, \lambda) \right| \lesssim |p_l|^{\frac{1}{2}+\varepsilon}, \quad l = 1, 2.$$

We emphasize, however, that this infrared assumption is required only in the case $\gamma_{lj} = 1$, that is, for $j = 1/2$. For all other $j \in \mathbb{N} + \frac{1}{2}$, we do *not* need to impose any infrared regularization on the generalized eigenstates $\psi_\pm((p, \gamma), x)$; They are already regular enough.
3) One verifies that Hypotheses 3.3(i) and 3.3(ii) imply Hypothesis 3.1.

Theorem 3.4 (Location of the spectrum). *Assume that Hypothesis* 3.3 *holds. There exists $g_1 > 0$ such that, for all $|g| \leq g_1$,*

$$\mathrm{Spec}(H_Z) = \{\inf \mathrm{Spec}(H_Z)\} \cup [\inf \mathrm{Spec}(H_Z) + \mathrm{m}_e, \infty).$$

In particular, H_Z has no eigenvalue below its essential spectrum except for the ground state energy, $\inf \mathrm{Spec}(H_Z)$, *which is an isolated simple eigenvalue.*

We use the Dereziński–Gérard partition of unity [16] in a version that accommodates the Fermi–Dirac statistics and the CAR. Such a partition of unity was used previously in [1] (see [9] for details).

Theorem 3.5 (Absolutely continuous spectrum). *Assume that Hypothesis* 3.3 *holds with* $\varepsilon > 0$ *in Hypothesis* 3.3(ii)*. For all* $\delta > 0$*, there exists* $g_\delta > 0$ *such that, for all* $|g| \leq g_\delta$*, the spectrum of* H_Z *in the interval*

$$[\inf \operatorname{Spec}(H_Z) + \mathrm{m}_e, \inf \operatorname{Spec}(H_Z) + \mathrm{m}_{Z^0} - \delta]$$

is purely absolutely continuous.

Ideas of the proof. The proof of Theorem 3.5 relies on Mourre positive commutator method. Though, the standard choice of a conjugate operator as the second quantized version of the one electron operator $\frac{1}{2}((\nabla_p \omega \cdot i\nabla_p + i\nabla_p \cdot (\nabla_p \omega))$ fails to give a Mourre estimate near thresholds, already for the free Hamiltonian $H_{Z,0}$.

Hence, we construct a conjugate operator A by following the idea of Hübner and Spohn [35] (see also [23, 24]). As in [35], the operator A is only maximal symmetric, and generates a C_0-semigroup of isometries. Therefore, we need to use Singular Mourre theory with non self-adjoint conjugate operator. Such extensions of the usual conjugate operator theory [38, 3] considered in [35] were later extended in [45] and in [23, 24].

The general strategy remains similar to the one using regular Mourre Theory. We prove regularity of the total Hamiltonian $H_{Z,I}$ with respect to the conjugate operator A. For this sake, we use here real interpolation theory together with a version of the Mourre theory requiring only low regularity of the Hamiltonian with respect to the conjugate operator (see [18] and [9, Appendix B]).

We then establish a Mourre estimate. Formally, our choice of the conjugate operator A yields $[H_{Z,0}, iA] = N_+ + N_-$, where $N_\pm$ are the number operators for electrons and positrons. Since $N_\pm \geq 1$ away from the vacuum, to obtain a strict Mourre inequality, it suffices to control $g[H_{Z,I}, iA]$ for g small enough. This is possible using general relative bounds with respect to $H_{Z,0}$ for perturbations of the form $H_{Z,I}(-iaF^{(\alpha)})$ (see (3.24)), for a denoting the one-particle conjugate operator, and $F^{(\alpha)}$ being the kernels given by (3.25).

Combining the Mourre estimate with a regularity property of the Hamiltonian with respect to the conjugate operator allow us to deduce a Virial theorem and a limiting absorption principle, from which we obtain Theorem 3.5.

Our main achievement consists in proving that the physical interaction Hamiltonian $H_{Z,I}$ is regular enough for the Mourre theory to be applied, except for the terms associated to the "first" generalized eigenstates ($j = 1/2$). For the latter, unfortunately, we need to impose a non-physical infrared condition. □

4. Prospectives

Despite the number of results concerning spectral and dynamical properties for weak interaction Hamiltonians or similar models, [7, 8, 2, 11, 13, 26, 4, 9, 10, 32, 33], the study of weak interactions from a rigorous point of view still requires to be investigated.

We mention here some open problems.

- *Spectral study above the boson thresholds.* To complete the spectral study of the above two models, it remains to prove that the spectrum above the massive bosons ($W^\pm$ or Z^0) thresholds is purely absolutely continuous, as expected for weak interactions models for which there should be no bound states except for the vacuum. Picking a conjugate operator including the massive bosons, i.e., a conjugate operator similar to the one we picked, with an additional term acting on the Bosonic Fock space, the general strategy adopted above is expected to give purely absolutely continuous spectrum away from bosonic thresholds. Near bosonic thresholds, like for instance near $(\inf \mathrm{Spec}(H_Z)) + \mathrm{m}_{Z^0}$ or $(\inf \mathrm{Spec}(H_W)) + \mathrm{m}_W$, we face some infrared problems. To obtain a limiting absorption principle near bosonic thresholds, it is expected, in the case of Z^0 decay, that one first has to derive local properties of the solutions of the Proca equation for massive spin 1 particles.
- *Weak decay of the intermediate boson Z into neutrinos and antineutrinos.* The decay of the Z^0,
$$Z^0 \to \nu_e + \bar{\nu}_e,$$
is apparently very similar to the model studied in Section 3. However, the two fermionic particles created in this process are massless, as described by the Standard Model. From a technical point of view, using conjugate operator theory with non self-adjoint conjugate operator as in Section 3 to prove absolutely continuity of the spectrum of the Hamiltonian H, yields additional difficulties in that case since, unlike for the model treated in Section 3, the commutator $[H, iA]$ is not comparable with H.
- *Decay of muonic atoms.* The decay of a free muon or of a muon in the electromagnetic field of a nucleus always produces more than three particles
$$\mu^- \to \nu_\mu + \bar{\nu}_e + e^-.$$
A natural way to describe this decay in muonic atoms, is to restrict the Fock space for muons to bound states of Dirac–Coulomb. Moreover, to account for high energies involved in this decay, it is sufficient to consider only free electron/positron states.

  The inherent mathematical difficulty is that we have to deal with a process with four fermionic particles, two of which are massless as given by the Standard Model. For this model, technical difficulties arise already for getting a relative bound with respect to the free Hamiltonian for the interaction. Without such a bound, it remains illusory with the current techniques to derive any interesting spectral properties.

- *Model with neutrino mass.* As mentioned in the introduction of Section 2, neutrinos (of the electrons, muons or tauons) have a mass. To account for this, one can add a mass to the neutrino in the model of Section 2. This model already gives interesting mathematical challenges, since the massive fermions "create" thresholds in the spectrum, but the masses of the neutrino are so tiny, that relative bounds can not be used as in Section 2 in the context of usual perturbative theory, unless dealing with interaction with irrelevant coupling constant $g \ll 1$.

  A physically more relevant way to take into account the neutrino mass is the study of Hamiltonians of post Standard Models.

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Magnetic Laplacian in Sharp Three-dimensional Cones

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Abstract. The core result of this paper is an upper bound for the ground state energy of the magnetic Laplacian with constant magnetic field on cones that are contained in a half-space. This bound involves a weighted norm of the magnetic field related to moments on a plane section of the cone. When the cone is sharp, i.e., when its section is small, this upper bound tends to 0. A lower bound on the essential spectrum is proved for families of sharp cones, implying that if the section is small enough the ground state energy is an eigenvalue. This circumstance produces corner concentration in the semiclassical limit for the magnetic Schrödinger operator when such sharp cones are involved.

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1. Introduction

1.1. Motivation

The onset of supraconductivity in presence of an intense magnetic field in a body occupying a domain Ω is related to the lowest eigenvalues of "semiclassical" magnetic Laplacians in Ω with natural boundary condition (see for instance [15, 9, 10]), and its localization is connected with the localization of the corresponding eigenfunctions.

The semiclassical expansion of the first eigenvalues of Neumann magnetic Laplacians has been addressed in numerous papers, considering constant or variable magnetic field. In order to introduce our present study, it is sufficient to discuss the case of a *constant magnetic field* $\mathbf{B}$ and of a simply connected domain Ω.

For any chosen $h > 0$, let us denote by $\lambda_h(\mathbf{B}, \Omega)$ the first eigenvalue of the magnetic Laplacian $(-ih\nabla + \mathbf{A})^2$ with Neumann boundary conditions. Here $\mathbf{A}$ is any associated potential (i.e., such that $\operatorname{curl} \mathbf{A} = \mathbf{B}$). The following facts are proved in dimension 2.

i) The eigenmodes associated with $\lambda_h(\mathbf{B}, \Omega)$ localize near the boundary as $h \to 0$, see [11].
ii) For a smooth boundary, these eigenmodes concentrate near the points of maximal curvature, see [8].
iii) In presence of corners for a polygonal domain, these eigenmodes localize near acute corners (i.e., of opening $\leq \frac{\pi}{2}$), see [2, 3].

Results i) and iii) rely on the investigation of the collection of the ground state energies $E(\mathbf{B}, \Pi_{\mathbf{x}})$ of the associated *tangent problems*, i.e., the magnetic Laplacians for $h = 1$ with the same magnetic field $\mathbf{B}$, posed on the (dilation invariant) tangent domains $\Pi_{\mathbf{x}}$ at each point $\mathbf{x}$ of the closure of Ω. The tangent domain $\Pi_{\mathbf{x}}$ is the full space $\mathbb{R}^2$ if $\mathbf{x}$ is an interior point, the half-space $\mathbb{R}^2_+$ if $\mathbf{x}$ belongs to a smooth part of the boundary $\partial\Omega$, and a sector $\mathcal{S}$ if $\mathbf{x}$ is a corner of a polygonal domain. The reason for i) is the inequality $E(\mathbf{B}, \mathbb{R}^2_+) < E(\mathbf{B}, \mathbb{R}^2)$ and the reason for iii) is that the ground state energy associated with an acute sector $\mathcal{S}$ is less than that of the half-plane $\mathbb{R}^2_+$. Beyond this result, there also holds the small angle asymptotics (see [2, Theorem 1.1]), with $\mathcal{S}_\alpha$ the sector of opening angle α,

$$E(\mathbf{B}, \mathcal{S}_\alpha) = \|\mathbf{B}\| \frac{\alpha}{\sqrt{3}} + \mathcal{O}(\alpha^3). \tag{1.1}$$

Asymptotic formulas for the first eigenvalue $\lambda_h(\mathbf{B}, \Omega)$ are established in various configurations (mainly in situations ii) and iii)) and the first term is always given by

$$\lim_{h \to 0} \frac{\lambda_h(\mathbf{B}, \Omega)}{h} = \inf_{\mathbf{x} \in \overline{\Omega}} E(\mathbf{B}, \Pi_{\mathbf{x}}) \,. \tag{1.2}$$

As far as three-dimensional domains are concerned, in the recent contribution [4] formula (1.2) is proved to be still valid in a general class of corner domains for which tangent domains at the boundary are either half-planes, infinite wedges or genuine infinite 3D cones with polygonal sections. Various convergence rates are proved. Thus the analysis of the Schrödinger operator with constant magnetic field on general cones is crucial to exhibit the main term of the expansion of the ground energy of the magnetic Laplacian in any corner domain. As in 2D, the interior case $\Pi_{\mathbf{x}} = \mathbb{R}^3$ ($\mathbf{x} \in \Omega$) is explicit, and the half-space is rather well known (see [16, 12]). The case of wedges has been more recently addressed in [17, 18, 19].

When the infimum is reached at a corner, a better upper bound of $\lambda_h(\mathbf{B}, \Omega)$ can be proved as soon as the bottom of the spectrum of the corresponding tangent operator is discrete [4, Theorem 9.1]. If, moreover, this infimum is attained *at corners only*, the corner concentration holds for associated eigenvectors [4, Section 12.1]. So the main motivation of the present paper is to investigate 3D cones in order to find sufficient conditions ensuring positive answers to the following questions:

(Q1) A 3D cone Π being given, does the energy $E(\mathbf{B},\Pi)$ correspond to a discrete eigenvalue for the associated magnetic Laplacian?

(Q2) A corner domain $\Omega \subset \mathbb{R}^3$ being given, is the infimum in (1.2) reached at a corner, or at corners only?

In [16], positive answers are given to these questions when Ω is a cuboid (so that the 3D tangent cones are octants), under some geometrical hypotheses on the orientation of the magnetic field. In [5, 6], the case of *right circular cones* (that we denote here by $\mathcal{C}^\circ_\alpha$ with α its opening) is investigated: a full asymptotics is proved, starting as

$$E(\mathbf{B},\mathcal{C}^\circ_\alpha) = \|\mathbf{B}\|\sqrt{1+\sin^2\beta}\,\frac{3\alpha}{4\sqrt{2}} + \mathcal{O}(\alpha^3), \tag{1.3}$$

where β is the angle between the magnetic field $\mathbf{B}$ and the axis of the cone. When combined with a positive α-independent lower bound of the essential spectrum, such an asymptotics guarantees that for α small enough, $E(\mathbf{B},\mathcal{C}^\circ_\alpha)$ is an eigenvalue, providing positive answer to Question (Q1).

The aim of this paper is to deal with more general cones, especially with *polygonal section*. We are going to prove an upper bound that has similar characteristics as the asymptotical term in (1.3). We will also prove that there exist eigenvalues below the essential spectrum as soon as the cone is *sharp* enough, and therefore provide sufficient conditions for a positive answer to Question (Q1).

One of the main new difficulties is that the essential spectrum strongly depends on the dihedral angles of the cones, and that, if these angles get small, the essential spectrum may go to 0 by virtue of the upper bound

$$E(\mathbf{B},\mathcal{W}_\alpha) \le \|\mathbf{B}\|\frac{\alpha}{\sqrt{3}} + \mathcal{O}(\alpha^3), \tag{1.4}$$

where α is the opening of the wedge $\mathcal{W}_\alpha$. Here the magnetic field $\mathbf{B}$ is assumed either to be contained in the bisector plane of the wedge (see [17, Proposition 7.6]), or to be tangent to a face of the wedge (see [18, Section 5]). The outcome of the present study is that eigenvalues will appear under the essential spectrum for sharp cones that do not have sharp edges.

Obviously, (1.4) may also be an obstruction to a positive answer to Question (Q2). Combining our upper bound for sharp cones with the positivity and the continuity of the ground energy on wedges, we will deduce that a domain that has a sharp corner gives a positive answer to (Q2), provided the opening of its edges remained bounded from below. We will also exhibit such a domain by an explicit construction.

Finally, we can mention that there exist in the literature various works dealing with spectral problems involving conical domains: Let us quote among others the "δ-interaction" Schrödinger operator, see [1], and the Robin Laplacian, see [14]. We find out that the latter problem shares many common features with the magnetic Laplacian, and will describe some of these analogies in the last section of our paper.

1.2. Main results

Let us provide now the framework and the main results of our paper. We will consider cones defined through a plane section.

Definition 1.1. Let ω be a bounded and connected open subset of $\mathbb{R}^2$. We define the cone $\mathcal{C}_\omega$ by

$$\mathcal{C}_\omega = \left\{ \mathbf{x} = (\mathsf{x}_1, \mathsf{x}_2, \mathsf{x}_3) \in \mathbb{R}^3 : \quad \mathsf{x}_3 > 0 \quad \text{and} \quad \left(\frac{\mathsf{x}_1}{\mathsf{x}_3}, \frac{\mathsf{x}_2}{\mathsf{x}_3} \right) \in \omega \right\}. \tag{1.5}$$

Let $\mathbf{B} = (\mathsf{B}_1, \mathsf{B}_2, \mathsf{B}_3)^\mathsf{T}$ be a constant magnetic field and $\mathbf{A}$ be an associated linear magnetic potential, i.e., such that $\operatorname{curl} \mathbf{A} = \mathbf{B}$. We consider the quadratic form

$$q[\mathbf{A}, \mathcal{C}_\omega](u) = \int_{\mathcal{C}_\omega} |(-i\nabla + \mathbf{A})u|^2 \, \mathrm{d}\mathbf{x},$$

defined on the form domain

$$\mathrm{Dom}(q[\mathbf{A}, \mathcal{C}_\omega]) = \left\{ u \in \mathrm{L}^2(\mathcal{C}_\omega) : \ (-i\nabla + \mathbf{A})u \in \mathrm{L}^2(\mathcal{C}_\omega) \right\}.$$

We denote by $H(\mathbf{A}, \mathcal{C}_\omega)$ the Friedrichs extension of this quadratic form. If the domain ω is regular enough (for example if ω is a bounded polygonal domain), $H(\mathbf{A}, \mathcal{C}_\omega)$ coincides with the Neumann realization of the magnetic Laplacian on $\mathcal{C}_\omega$ with the magnetic field $\mathbf{B}$. By gauge invariance the spectrum of $H(\mathbf{A}, \mathcal{C}_\omega)$ depends only on the magnetic field $\mathbf{B}$ and not on the magnetic potential $\mathbf{A}$ that is *a priori* assumed to be linear. For $n \in \mathbb{N}$, we define $E_n(\mathbf{B}, \mathcal{C}_\omega)$ as the nth Rayleigh quotient of $H(\mathbf{A}, \mathcal{C}_\omega)$:

$$E_n(\mathbf{B}, \mathcal{C}_\omega) = \sup_{u_1, \ldots, u_{n-1} \in \mathrm{Dom}(q[\mathbf{A}, \mathcal{C}_\omega])} \ \inf_{\substack{u \in [u_1, \ldots, u_{n-1}]^\perp \\ u \in \mathrm{Dom}(q[\mathbf{A}, \mathcal{C}_\omega])}} \frac{q[\mathbf{A}, \mathcal{C}_\omega](u)}{\|u\|^2_{\mathrm{L}^2(\mathcal{C}_\omega)}}. \tag{1.6}$$

For $n = 1$, we shorten the notation by $E(\mathbf{B}, \mathcal{C}_\omega)$ that is the ground state energy of the magnetic Laplacian $H(\mathbf{A}, \mathcal{C}_\omega)$.

1.2.1. Upper bound for the first Rayleigh quotients. Our first result states an upper bound for $E_n(\mathbf{B}, \mathcal{C}_\omega)$ valid for any section ω.

Theorem 1.2. *Let ω be an open bounded subset of $\mathbb{R}^2$ and $\mathbf{B}$ be a constant magnetic field. We define, for $k = 0, 1, 2$, the normalized moments (here $|\omega|$ denotes the measure of ω)*

$$m_k := \frac{1}{|\omega|} \int_\omega \mathsf{x}_1^k \mathsf{x}_2^{2-k} \, \mathrm{d}\mathsf{x}_1 \, \mathrm{d}\mathsf{x}_2.$$

The nth Rayleigh quotient satisfies the upper bound

$$E_n(\mathbf{B}, \mathcal{C}_\omega) \leq (4n - 1) e(\mathbf{B}, \omega), \tag{1.7}$$

where $e(\mathbf{B}, \omega)$ is the positive constant defined by

$$e(\mathbf{B}, \omega) = \left(\mathsf{B}_3^2 \frac{m_0 m_2 - m_1^2}{m_0 + m_2} + \mathsf{B}_2^2 m_2 + \mathsf{B}_1^2 m_0 - 2\mathsf{B}_1 \mathsf{B}_2 m_1 \right)^{1/2}. \tag{1.8}$$

Lemma 1.3. *There holds*

i) *The application* $\mathbf{B} \mapsto e(\mathbf{B}, \omega)$ *is an* ω*-dependent norm on* $\mathbb{R}^3$.
ii) *The application* $(\mathbf{B}, \omega) \mapsto e(\mathbf{B}, \omega)$ *is homogeneous:*

$$e(\mathbf{B}, \omega) = |\omega|^{1/2} \, \|\mathbf{B}\| \; e(\mathbf{b}, \varpi), \qquad \textit{with} \qquad \mathbf{b} = \frac{\mathbf{B}}{\|\mathbf{B}\|}, \quad \varpi = \frac{\omega}{|\omega|}. \tag{1.9}$$

Remark 1.4. a) Although the quantity $e(\mathbf{B}, \omega)$ is independent of the choice of the Cartesian coordinates $(\mathsf{x}_1, \mathsf{x}_2)$ in the plane $\mathsf{x}_3 = 0$, it strongly depends on the choice of the x_3 "axis" defining this plane. Indeed, if a cone $\mathcal{C}$ contained in a half-space is given, there are many different choices possible for coordinates $(\mathsf{x}_1, \mathsf{x}_2, \mathsf{x}_3)$ so that $\mathcal{C}$ can be represented as (1.5). To each choice of the x_3 axis corresponds a distinct definition of ω. For instance, let $\mathcal{C}$ be a circular cone. If the x_3 axis is chosen as the axis of the cone, then ω is a disc. Any different choice of the axis x_3 yields an ellipse for ω and the corresponding quantity $e(\mathbf{B}, \omega)$ would be larger.

b) When ω is the disc of center $(0,0)$ and radius $\tan \frac{\alpha}{2}$, the cone $\mathcal{C}_\omega$ equals the circular cone $\mathcal{C}^\circ_\alpha$ of opening α considered in [5, 6]. Then we find that $e(\mathbf{B}, \omega)$ coincides with the first term of the asymptotics (1.3) modulo $\mathcal{O}(\alpha^3)$, which proves that our upper bound is sharp in this case (see Section 3.2.1 below).

1.2.2. Convergence of the bottom of essential spectrum. By the min-max principle, the quantity $E_n(\mathbf{B}, \mathcal{C}_\omega)$, defined in (1.6), is either the nth eigenvalue of $H(\mathbf{A}, \mathcal{C}_\omega)$, or the bottom of the essential spectrum denoted by $E_{\text{ess}}(\mathbf{B}, \mathcal{C}_\omega)$.

The second step of our investigation is then to determine the bottom of the essential spectrum. We assume that ω is a bounded polygonal domain in $\mathbb{R}^2$. This means that the boundary of ω is a finite union of smooth arcs (the sides) and that the tangents to two neighboring sides at their common end (a vertex) are not colinear. Then the set $\mathcal{C}_\omega \cap \mathbb{S}^2$ called the section of the cone $\mathcal{C}_\omega$ is a polygonal domain of the sphere that has the same properties. For any $\mathbf{p} \in \overline{\mathcal{C}_\omega} \cap \mathbb{S}^2$, we denote by $\Pi_{\mathbf{p}} \subset \mathbb{R}^3$ the tangent cone to $\mathcal{C}_\omega$ at $\mathbf{p}$. More details about the precise definition of a tangent cone can be found in the Appendix or in [4, Section 3]. Let us now describe the nature of $\Pi_{\mathbf{p}}$ according to the location of $\mathbf{p}$ in the section of $\overline{\mathcal{C}_\omega}$:

(a) If $\mathbf{p}$ belongs to $\mathcal{C}_\omega \cap \mathbb{S}^2$, i.e., is an interior point, then $\Pi_{\mathbf{p}} = \mathbb{R}^3$.
(b) If $\mathbf{p}$ belongs to the regular part of the boundary of $\mathcal{C}_\omega \cap \mathbb{S}^2$ (that is if $\mathbf{p}$ is in the interior of a side of $\mathcal{C}_\omega \cap \mathbb{S}^2$), then $\Pi_{\mathbf{p}}$ is a half-space.
(c) If $\mathbf{p}$ is a vertex of $\mathcal{C}_\omega \cap \mathbb{S}^2$ of opening θ, then $\Pi_{\mathbf{p}}$ is a wedge of opening θ.

The cone $\Pi_{\mathbf{p}}$ is called a tangent substructure of $\mathcal{C}_\omega$. The ground state energy of the magnetic Laplacian on $\Pi_{\mathbf{p}}$ with magnetic field $\mathbf{B}$ is well defined and still denoted by $E(\mathbf{B}, \Pi_{\mathbf{p}})$. Let us introduce the infimum of the ground state energies on the tangent substructures of $\mathcal{C}_\omega$:

$$\mathscr{E}^*(\mathbf{B}, \mathcal{C}_\omega) := \inf_{\mathbf{p} \in \overline{\mathcal{C}_\omega} \cap \mathbb{S}^2} E(\mathbf{B}, \Pi_{\mathbf{p}}). \tag{1.10}$$

Then [4, Theorem 6.6] yields that the bottom of the essential spectrum $E_{\text{ess}}(\mathbf{B}, \mathcal{C}_\omega)$ of the operator $H(\mathbf{A}, \mathcal{C}_\omega)$ is given by this quantity:

$$E_{\text{ess}}(\mathbf{B}, \mathcal{C}_\omega) = \mathscr{E}^*(\mathbf{B}, \mathcal{C}_\omega). \tag{1.11}$$

Now we take the view point of small angle asymptotics, like in (1.1), (1.3), and (1.4). But for general 3D cones there is no obvious notion of small angle α. That is why we introduce families of sharp cones for which the plane section ω is scaled by a small parameter $\varepsilon > 0$. More precisely, $\omega \subset \mathbb{R}^2$ being given, we define the dilated domain

$$\omega_\varepsilon := \varepsilon\omega, \quad \varepsilon > 0, \tag{1.12}$$

and consider the family of cones $\mathcal{C}_{\omega_\varepsilon}$ parametrized by (1.12), as $\varepsilon \to 0$. The homogeneity (1.9) of the bound $e(\mathbf{B}, \omega)$ implies immediately

$$e(\mathbf{B}, \omega_\varepsilon) = e(\mathbf{B}, \omega)\, \varepsilon\, . \tag{1.13}$$

Thus the bound (1.7) implies that the Rayleigh quotients $E_n(\mathbf{B}, \mathcal{C}_{\omega_\varepsilon})$ tend to 0 as $\varepsilon \to 0$.

To determine the asymptotic behavior of $E_{\text{ess}}(\mathbf{B}, \mathcal{C}_{\omega_\varepsilon})$ as $\varepsilon \to 0$, we introduce $\widehat{\omega}$ as the cylinder $\omega \times \mathbb{R}$ and define the infimum of ground energies

$$\mathscr{E}(\mathbf{B}, \widehat{\omega}) = \inf_{\mathbf{x}' \in \overline{\omega}} E(\mathbf{B}, \widehat{\Pi}_{(\mathbf{x}',1)}),$$

where, for $\mathbf{x}$ in the closure of $\widehat{\omega}$, $\widehat{\Pi}_{\mathbf{x}}$ denotes the tangent cone to $\widehat{\omega}$ at $\mathbf{x}$. We note that, by translation invariance along the third coordinate, $\mathscr{E}(\mathbf{B}, \widehat{\omega})$ is also the infimum of ground energies when $\mathbf{x}$ varies in the whole cylinder $\overline{\widehat{\omega}}$.

Proposition 1.5. *Let ω be a bounded polygonal domain of $\mathbb{R}^2$, and ω_ε defined by* (1.12). *Then*

$$\lim_{\varepsilon \to 0} E_{\text{ess}}(\mathbf{B}, \mathcal{C}_{\omega_\varepsilon}) = \mathscr{E}(\mathbf{B}, \widehat{\omega}) > 0.$$

Taking (1.13) into account, as a direct consequence of Theorem 1.2 and Proposition 1.5, we deduce:

Corollary 1.6. *Let ω be a bounded polygonal domain of $\mathbb{R}^2$ and $\mathbf{B}$ be a constant magnetic field. For all $n \geq 1$, for all $\varepsilon > 0$, there holds*

$$E_n(\mathbf{B}, \mathcal{C}_{\omega_\varepsilon}) \leq (4n-1)e(\mathbf{B}, \omega)\varepsilon.$$

In particular, for ε small enough, there exists an eigenvalue below the essential spectrum.

Remark 1.7. It is far from being clear whether $(4n-1)e(\mathbf{B}, \omega)\varepsilon$ can be the first term of an eigenvalue asymptotics, like this is the case for circular cones as proved in [5, 6].

1.2.3. Corner concentration in the semiclassical framework. Let $\Omega \subset \mathbb{R}^3$ be a bounded simply connected corner domain in the sense of Definition A.2 (see [4, Section 3] for more details). We denote by $H_h(\mathbf{A}, \Omega)$ the Neumann realization of the Schrödinger operator $(-ih\nabla + \mathbf{A})^2$ on Ω with magnetic potential $\mathbf{A}$ and semiclassical parameter h. Due to gauge invariance, its eigenvalues depend on the magnetic field $\mathbf{B} = \operatorname{curl} \mathbf{A}$, and not on the potential $\mathbf{A}$, whereas the eigenfunctions do depend on $\mathbf{A}$. We are interested in the first eigenvalue $\lambda_h(\mathbf{B}, \Omega)$ of $H_h(\mathbf{A}, \Omega)$ and in associated normalized eigenvector $\psi_h(\mathbf{A}, \Omega)$.

Let us briefly recall some of the results of [4], restricting the discussion to the case when the *magnetic field* $\mathbf{B}$ *is constant* (and $\mathbf{A}$ linear) for simplicity of exposition. To each point $\mathbf{x} \in \overline{\Omega}$ is associated with a dilation invariant, tangent open set $\Pi_{\mathbf{x}}$, according to the following cases:

1. If $\mathbf{x}$ is an interior point, $\Pi_{\mathbf{x}} = \mathbb{R}^3$,
2. If $\mathbf{x}$ belongs to a *face* $\mathbf{f}$ (*i.e.*, a connected component of the smooth part of $\partial\Omega$), $\Pi_{\mathbf{x}}$ is a half-space,
3. If $\mathbf{x}$ belongs to an *edge* $\mathbf{e}$, $\Pi_{\mathbf{x}}$ is an infinite wedge,
4. If $\mathbf{x}$ is a *vertex* $\mathbf{v}$, $\Pi_{\mathbf{x}}$ is an infinite cone.

The *local energy* $E(\mathbf{B}, \Pi_{\mathbf{x}})$ at $\mathbf{x}$ is defined as the ground energy of the tangent operator $H(\mathbf{A}, \Pi_{\mathbf{x}})$ and the *lowest local energy* is written as

$$\mathscr{E}(\mathbf{B}, \Omega) := \inf_{\mathbf{x} \in \overline{\Omega}} E(\mathbf{B}, \Pi_{\mathbf{x}}). \tag{1.14}$$

Then [4, Theorem 5.1 & 9.1] provides the general asymptotical bounds

$$|\lambda_h(\mathbf{B}, \Omega) - h\mathscr{E}(\mathbf{B}, \Omega)| \leq C\, h^{11/10} \quad \text{as} \quad h \to 0\ . \tag{1.15}$$

Let $E_{\mathrm{ess}}(\mathbf{B}, \Pi_{\mathbf{x}})$ be the bottom of the essential spectrum of $H(\mathbf{A}, \Pi_{\mathbf{x}})$. If there exists a vertex $\mathbf{v}$ of Ω such that

$$\mathscr{E}(\mathbf{B}, \Omega) = E(\mathbf{B}, \Pi_{\mathbf{v}}) < E_{\mathrm{ess}}(\mathbf{B}, \Pi_{\mathbf{v}}), \tag{1.16}$$

then there holds the improved upper bound $\lambda_h(\mathbf{B}, \Omega) \leq h\mathscr{E}(\mathbf{B}, \Omega) + C\, h^{3/2}|\log h|$, see [4, Theorem 9.1 (d)]. Finally, if the lowest local energy is attained at vertices only, in the following strong sense (here $\mathfrak{V}$ is the set of vertices of Ω)

$$\mathscr{E}(\mathbf{B}, \Omega) < \inf_{\mathbf{x} \in \overline{\Omega} \setminus \mathfrak{V}} E(\mathbf{B}, \Pi_{\mathbf{x}}), \tag{1.17}$$

the first eigenvalue $\lambda_h(\mathbf{B}, \Omega)$ has an asymptotic expansion as $h \to 0$ ensuring the improved bounds

$$|\lambda_h(\mathbf{B}, \Omega) - h\mathscr{E}(\mathbf{B}, \Omega)| \leq C\, h^{3/2} \quad \text{as} \quad h \to 0\ , \tag{1.18}$$

and, moreover, the corresponding eigenfunction concentrates near the vertices $\mathbf{v}$ such that $\mathscr{E}(\mathbf{B}, \Omega) = E(\mathbf{B}, \Pi_{\mathbf{v}})$. This is an immediate adaptation of [3] to the 3D case, see [4, Section 12.1]. In this framework, our result is now

Proposition 1.8. *Let ω be a bounded polygonal domain of $\mathbb{R}^2$, and ω_ε defined by* (1.12).

a) *Let $\big(\Omega(\varepsilon)\big)_\varepsilon$ be a family of* 3D *corner domains such that*

i) *One of the vertices* $\mathbf{v}(\varepsilon)$ *of* $\Omega(\varepsilon)$ *satisfies* $\Pi_{\mathbf{v}(\varepsilon)} = \mathcal{C}_{\omega_\varepsilon}$,

ii) *The edge openings* $\alpha_{\mathbf{x}}$ *of all domains* $\Omega(\varepsilon)$ *satisfy the uniform bounds*

$$\beta_0 \leq \alpha_{\mathbf{x}} \leq 2\pi - \beta_0, \quad \forall \mathbf{x} \text{ edge point of } \Omega(\varepsilon), \ \forall \varepsilon > 0, \tag{1.19}$$

with a positive constant β_0.

Then condition (1.17) *is satisfied for* ε *small enough.*

b) *Families* $\big(\Omega(\varepsilon)\big)_\varepsilon$ *satisfying the above assumptions* i) *and* ii) *do exist.*

1.2.4. Outline of the paper. The paper is organized as follows: Sections 2–3 are devoted to the proof of Theorem 1.2: To get an upper bound of $E_n(\mathbf{B}, \mathcal{C}_\omega)$, we introduce in Section 2 a reduced operator on the half-line, depending on the chosen axis $\mathsf{x}_3 > 0$, and introduce test functions for the reduced Rayleigh quotients. Then, in Section 3, we optimize the choice of the magnetic potential $\mathbf{A}$ in order to minimize the reduced Rayleigh quotients. The obtained upper bounds are explicitly computed in some examples like discs and rectangles. In Section 4, we focus on the essential spectrum for a sharp cone $\mathcal{C}_{\omega_\varepsilon}$ with polygonal section and prove Proposition 4.1 that is a stronger form of Proposition 1.5. Section 5 is devoted to the proof of Proposition 1.8 that provides cases of corner concentration for the first eigenvectors of the semiclassical magnetic Laplacian. We conclude the paper in Section 6 by a comparison with Robin problem. Finally, for completeness, we recall in the Appendix the recursive definition of corner domains.

2. Upper bound for the first Rayleigh quotients using a 1D operator

The aim of the two following sections is to establish an upper bound of the nth Rayleigh quotient $E_n(\mathbf{B}, \mathcal{C}_\omega)$, valid for any domain ω.

For any constant magnetic potential $\mathbf{B}$, we introduce the subspace

$$\mathcal{A}(\mathbf{B}) = \{\mathbf{A} \in \mathcal{L}(\mathbb{R}^3) : \quad \partial_{\mathsf{x}_3}\mathbf{A} = 0 \quad \text{and} \quad \nabla \times \mathbf{A} = \mathbf{B}\},$$

where $\mathcal{L}(\mathbb{R}^3)$ denotes the set of the endomorphisms of $\mathbb{R}^3$. The set $\mathcal{A}(\mathbf{B})$ is not empty and we can consider $\mathbf{A} \in \mathcal{A}(\mathbf{B})$. Let ω be a bounded polygonal domain. We evaluate now the quadratic form $q[\mathbf{A}, \mathcal{C}_\omega](\varphi)$ for functions φ only depending on the x_3 variable. This leads to introduce a new quadratic form on some weighted Hilbert space.

Lemma 2.1. *Let us introduce the weighted space* $\mathrm{L}^2_{\mathrm{w}}(\mathbb{R}_+) := \mathrm{L}^2(\mathbb{R}_+, \mathsf{x}^2\,\mathrm{d}\mathsf{x})$ *endowed with the norm* $\|u\|_{\mathrm{L}^2_{\mathrm{w}}(\mathbb{R}_+)} := \Big(\int_{\mathbb{R}_+} |u(\mathsf{x})|^2 \mathsf{x}^2\,\mathrm{d}\mathsf{x}\Big)^{1/2}$. *For any parameter* $\lambda > 0$, *we define the quadratic form* $\mathfrak{p}[\lambda]$ *by*

$$\mathfrak{p}[\lambda](u) = \int_{\mathbb{R}_+} \big(|u'(\mathsf{x})|^2 + \lambda \mathsf{x}^2 |u(\mathsf{x})|^2\big)\,\mathsf{x}^2\,\mathrm{d}\mathsf{x},$$

on the domain $\mathrm{B}_{\mathrm{w}}(\mathbb{R}_+) := \{u \in \mathrm{L}^2_{\mathrm{w}}(\mathbb{R}_+) : \mathsf{x}u \in \mathrm{L}^2_{\mathrm{w}}(\mathbb{R}_+), u' \in \mathrm{L}^2_{\mathrm{w}}(\mathbb{R}_+)\}$.

Let $\mathbf{A} \in \mathcal{A}(\mathbf{B})$ *and* $\varphi \in \mathrm{B_w}(\mathbb{R}_+)$. *Then the function* $\mathcal{C}_\omega \ni \mathbf{x} \mapsto \varphi(\mathsf{x}_3)$, *still denoted by* φ, *belongs to* $\mathrm{Dom}(q[\mathbf{A}, \mathcal{C}_\omega])$. *Moreover there holds*

$$\frac{q[\mathbf{A}, \mathcal{C}_\omega](\varphi)}{\|\varphi\|^2_{\mathrm{L}^2(\mathcal{C}_\omega)}} = \frac{\mathfrak{p}[\lambda](\varphi)}{\|\varphi\|^2_{\mathrm{L}^2_\mathrm{w}(\mathbb{R}_+)}} \qquad \textit{with} \qquad \lambda = \frac{\|\mathbf{A}\|^2_{\mathrm{L}^2(\omega)}}{|\omega|}.$$

Proof. Let $\mathbf{A} = (\mathsf{A}_1, \mathsf{A}_2, \mathsf{A}_3)^\mathsf{T} \in \mathcal{A}(\mathbf{B})$. Since φ is real-valued and depends only on the x_3 variable, we have

$$\begin{aligned} q[\mathbf{A}, \mathcal{C}_\omega](\varphi) &= \int_{\mathcal{C}_\omega} |\mathsf{A}_1|^2|\varphi|^2 + |\mathsf{A}_2|^2|\varphi|^2 + |(-i\partial_{\mathsf{x}_3} + \mathsf{A}_3)\varphi|^2 \,\mathrm{d}\mathbf{x} \\ &= \int_{\mathcal{C}_\omega} |\mathbf{A}(\mathbf{x})|^2|\varphi(\mathsf{x}_3)|^2 + |\partial_{\mathsf{x}_3}\varphi(\mathsf{x}_3)|^2 \,\mathrm{d}\mathbf{x}. \end{aligned}$$

Let us perform the change of variables

$$\mathbf{X} = (\mathsf{X}_1, \mathsf{X}_2, \mathsf{X}_3) = \left(\frac{\mathsf{x}_1}{\mathsf{x}_3}, \frac{\mathsf{x}_2}{\mathsf{x}_3}, \mathsf{x}_3\right). \tag{2.1}$$

Since $\mathbf{A}$ is linear and does not depends on x_3, we have

$$\begin{aligned} q[\mathbf{A}, \mathcal{C}_\omega](\varphi) &= \int_{\omega\times\mathbb{R}+} \Big(|\mathbf{A}(\mathbf{X})|^2\mathsf{X}_3^2|\varphi(\mathsf{X}_3)|^2 + |\varphi'(\mathsf{X}_3)|^2\Big)\mathsf{X}_3^2 \,\mathrm{d}\mathbf{X} \\ &= |\omega| \int_{\mathbb{R}+} |\varphi'(\mathsf{X}_3)|^2\mathsf{X}_3^2 \,\mathrm{d}\mathsf{X}_3 + \|\mathbf{A}\|^2_{\mathrm{L}^2(\omega)} \int_{\mathbb{R}+} |\varphi(\mathsf{X}_3)|^2\mathsf{X}_3^4 \,\mathrm{d}\mathsf{X}_3, \end{aligned}$$

and, with the same change of variables (2.1)

$$\|\varphi\|^2_{\mathrm{L}^2(\mathcal{C}_\omega)} \quad = \quad |\omega| \int_{\mathbb{R}+} |\varphi(\mathsf{X}_3)|^2\mathsf{X}_3^2 \,\mathrm{d}\mathsf{X}_3.$$

Thus the Rayleigh quotient is written

$$\frac{q[\mathbf{A}, \mathcal{C}_\omega](\varphi)}{\|\varphi\|^2_{\mathrm{L}^2(\mathcal{C}_\omega)}} = \frac{\int_{\mathbb{R}+} |\varphi'(\mathsf{X}_3)|^2\mathsf{X}_3^2 \,\mathrm{d}\mathsf{X}_3 + \frac{\|\mathbf{A}\|^2_{\mathrm{L}^2(\omega)}}{|\omega|} \int_{\mathbb{R}+} |\varphi(\mathsf{X}_3)|^2\mathsf{X}_3^4 \,\mathrm{d}\mathsf{X}_3}{\int_{\mathbb{R}+} |\varphi(\mathsf{X}_3)|^2 X_3^2 \,\mathrm{d}\mathsf{X}_3},$$

and we deduce the lemma. □

With Lemma 2.1 at hands, we are interested in the spectrum of the operator associated with the quadratic form $\mathfrak{p}[\lambda]$. Thanks to the change of function $u \mapsto U := \mathsf{x}u$, the weight is eliminated and we find by using an integration by parts that

$$\mathfrak{p}[\lambda](u) = \int_{\mathbb{R}_+} \left(|U'(\mathsf{x})|^2 + \lambda\mathsf{x}^2|U(\mathsf{x})|^2\right) \,\mathrm{d}\mathsf{x} \quad \text{and} \quad \|u\|^2_{\mathrm{L}^2_\mathrm{w}(\mathbb{R}_+)} = \|U\|^2_{\mathrm{L}^2(\mathbb{R}_+)}.$$

So we are reduced to a harmonic oscillator on $\mathbb{R}_+$ with Dirichlet condition at 0. Its eigenvectors U_n are the restrictions to $\mathbb{R}_+$ of the odd ones on $\mathbb{R}$. Therefore, see also [5, Corollary C.2], we find that the eigenvalues of the operator associated with the form $\mathfrak{p}[\lambda]$ are simple and the nth eigenvalue equals $\lambda^{1/2}(4n-1)$. Then, by combining the min-max principle with Lemma 2.1, we deduce that the nth eigenvalue of the operator associated with the form $q[\mathbf{A}, \mathcal{C}_\omega]$ is bounded from above by $(4n-1)\|\mathbf{A}\|_{\mathrm{L}^2(\omega)}/\sqrt{|\omega|}$. Since this upper bound is valid for any $\mathbf{A} \in \mathcal{A}(\mathbf{B})$, we have proved the following proposition.

Proposition 2.2. *Let* $\mathbf{B}$ *be a constant magnetic field. Then for all* $n \in \mathbb{N}^*$, *we have*

$$E_n(\mathbf{B}, \mathcal{C}_\omega) \leq \frac{4n-1}{\sqrt{|\omega|}} \inf_{\mathbf{A}\in\mathcal{A}(\mathbf{B})} \|\mathbf{A}\|_{\mathrm{L}^2(\omega)}, \tag{2.2}$$

with

$$\mathcal{A}(\mathbf{B}) = \{\mathbf{A} \in \mathcal{L}(\mathbb{R}^3) : \quad \partial_{\mathsf{x}_3}\mathbf{A} = 0 \quad \text{and} \quad \nabla \times \mathbf{A} = \mathbf{B}\}.$$

3. Optimization

The aim of this section is to give an explicit solution to the optimization problem

$$\textit{Find} \ \ \mathbf{A}_0 \in \mathcal{A}(\mathbf{B}) \ \ \textit{such that} \quad \|\mathbf{A}_0\|_{\mathrm{L}^2(\omega)} = \inf_{\mathbf{A}\in\mathcal{A}(\mathbf{B})} \|\mathbf{A}\|_{\mathrm{L}^2(\omega)}, \tag{3.1}$$

for a constant magnetic field $\mathbf{B} = (\mathsf{B}_1, \mathsf{B}_2, \mathsf{B}_3)^{\mathsf{T}}$. We also provide explicit examples in the case where the domain ω is a disc or a rectangle.

3.1. Resolution of the optimization problem and proof of Theorem 1.2

Let $\mathbf{A} = (\mathsf{A}_1, \mathsf{A}_2, \mathsf{A}_3)^{\mathsf{T}} \in \mathcal{A}(\mathbf{B})$. Since $\mathbf{A}$ is independent of the x_3 variable, we have

$$\operatorname{curl}\mathbf{A} = \begin{pmatrix} \partial_{\mathsf{x}_2}\mathsf{A}_3 \\ -\partial_{\mathsf{x}_1}\mathsf{A}_3 \\ \partial_{\mathsf{x}_1}\mathsf{A}_2 - \partial_{\mathsf{x}_2}\mathsf{A}_1 \end{pmatrix} = \begin{pmatrix} \mathsf{B}_1 \\ \mathsf{B}_2 \\ \mathsf{B}_3 \end{pmatrix}.$$

By linearity of $\mathbf{A}$, we have necessarily $\mathsf{A}_3(\mathbf{x}) = \mathsf{B}_1\mathsf{x}_2 - \mathsf{B}_2\mathsf{x}_1$. Therefore considering

$$\mathcal{A}' = \{\mathbf{A}' \in \mathcal{L}(\mathbb{R}^2) : \quad \nabla_{\mathsf{x}_1,\mathsf{x}_2} \times \mathbf{A}' = 1\},$$

the infimum in (3.1) is written

$$\inf_{\mathbf{A}\in\mathcal{A}(\mathbf{B})} \|\mathbf{A}\|_{\mathrm{L}^2(\omega)} = \left(\mathsf{B}_3^2 \inf_{\mathbf{A}'\in\mathcal{A}'} \|\mathbf{A}'\|^2_{\mathrm{L}^2(\omega)} + \int_\omega (\mathsf{B}_1\mathsf{x}_2 - \mathsf{B}_2\mathsf{x}_1)^2 \,\mathrm{d}\mathsf{x}_1\,\mathrm{d}\mathsf{x}_2\right)^{1/2}, \tag{3.2}$$

and 3D optimization problem (3.1) can be reduced to a 2D one:

$$\textit{Find} \ \ \mathbf{A}'_0 \in \mathcal{A}' \ \ \textit{such that} \quad \|\mathbf{A}'_0\|_{\mathrm{L}^2(\omega)} = \inf_{\mathbf{A}'\in\mathcal{A}'} \|\mathbf{A}'\|_{\mathrm{L}^2(\omega)}. \tag{3.3}$$

This problem can be solved explicitly:

Proposition 3.1. *For* $k = 0, 1, 2$, *we define the moments*

$$M_k := \int_\omega \mathsf{x}_1^k \mathsf{x}_2^{2-k} \,\mathrm{d}\mathsf{x}_1\,\mathrm{d}\mathsf{x}_2.$$

Then, we have

$$\inf_{\mathbf{A}'\in\mathcal{A}'} \|\mathbf{A}'\|^2_{\mathrm{L}^2(\omega)} = \frac{M_0M_2 - M_1^2}{M_0 + M_2}.$$

Moreover the minimizer of (3.3) *exists, is unique, and given by*

$$\mathbf{A}'_0(\mathsf{x}_1, \mathsf{x}_2) = \frac{1}{M_0 + M_2} \begin{pmatrix} M_1 & -M_0 \\ M_2 & -M_1 \end{pmatrix} \begin{pmatrix} \mathsf{x}_1 \\ \mathsf{x}_2 \end{pmatrix}.$$

Remark 3.2.

a) Let us notice that

$$M_0M_2 - M_1^2 = \frac{1}{2}\int_\omega\int_\omega (\mathsf{x}_1\mathsf{x}_2' - \mathsf{x}_1'\mathsf{x}_2)^2 \,\mathrm{d}\mathsf{x}_1\,\mathrm{d}\mathsf{x}_2\,\mathrm{d}\mathsf{x}_1'\,\mathrm{d}\mathsf{x}_2'.$$

This relation highlights once more the connection with he geometry of ω.

b) The divergence of the optimal transverse potential $\mathbf{A}_0'$ is 0, just as the full associated potential $\mathbf{A}_0$.

Proof. Let us introduce the space of linear applications of the plane $\mathcal{L}(\mathbb{R}^2)$ endowed with the scalar product

$$\langle f, g\rangle_{\mathrm{L}^2(\omega)} = \int_\omega f(\mathsf{x}_1,\mathsf{x}_2)\cdot g(\mathsf{x}_1,\mathsf{x}_2)\,\mathrm{d}\mathsf{x}_1\,\mathrm{d}\mathsf{x}_2, \qquad \forall f,g\in\mathcal{L}(\mathbb{R}^2).$$

Then $\mathcal{A}'$ is an affine hyperplane of $\mathcal{L}(\mathbb{R}^2)$ of dimension 3, and Problem (3.3) is equivalent to find the distance from the origin $\mathbf{0}$ to this hyperplane. In particular there exists a unique minimizer to (3.3), which is the orthogonal projection of $\mathbf{0}$ to $\mathcal{A}'$. To make the solution explicit, we look for a linear function $\mathbf{A}_0' \in \mathcal{A}'$ of the form

$$\mathbf{A}_0'(\mathsf{x}_1,\mathsf{x}_2) = \begin{pmatrix} \alpha & \beta \\ 1+\beta & \gamma \end{pmatrix}\begin{pmatrix} \mathsf{x}_1 \\ \mathsf{x}_2 \end{pmatrix},$$

where (α,β,γ) are to be found. Then we have

$$\begin{aligned} F(\alpha,\beta,\gamma) := \|\mathbf{A}_0'\|^2_{\mathrm{L}^2(\omega)} &= \int_\omega (\alpha\mathsf{x}_1+\beta\mathsf{x}_2)^2 + ((1+\beta)\mathsf{x}_1+\gamma\mathsf{x}_2)^2\,\mathrm{d}\mathsf{x}_1\,\mathrm{d}\mathsf{x}_2 \\ &= M_2(\alpha^2+(1+\beta)^2) + 2M_1(\alpha\beta+(1+\beta)\gamma) + M_0(\beta^2+\gamma^2). \end{aligned}$$

Solving $\nabla F = 0$ gives a unique solution

$$(\alpha,\beta,\gamma) = \frac{1}{M_0+M_2}(M_1,-M_0,-M_1),$$

and computations provide

$$\|\mathbf{A}_0'\|^2_{\mathrm{L}^2(\omega)} = \frac{M_0M_2-M_1^2}{M_0+M_2}.$$

We deduce the proposition. □

Proof of Theorem 1.2. Now, combining Proposition 2.2, (3.2) and Proposition 3.1, we get the upper bound

$$E_n(\mathbf{B},\mathcal{C}_\omega) \le (4n-1)e(\mathbf{B},\mathcal{C}_\omega),$$

with

$$\begin{aligned} e(\mathbf{B},\omega) &= \frac{1}{\sqrt{|\omega|}}\left(\mathsf{B}_3^2\frac{M_0M_2-M_1^2}{M_0+M_2} + \int_\omega (\mathsf{x}_1\mathsf{B}_2-\mathsf{B}_2\mathsf{x}_1)^2\,\mathrm{d}\mathsf{x}_1\,\mathrm{d}\mathsf{x}_2\right)^{1/2} \\ &= \frac{1}{\sqrt{|\omega|}}\left(\mathsf{B}_3^2\frac{M_0M_2-M_1^2}{M_0+M_2} + \mathsf{B}_2^2M_2 + \mathsf{B}_1^2M_0 - 2\mathsf{B}_1\mathsf{B}_2M_1\right)^{1/2} \end{aligned}$$

$$= \left(\mathsf{B}_3^2 \frac{m_0 m_2 - m_1^2}{m_0 + m_2} + \mathsf{B}_2^2 m_2 + \mathsf{B}_1^2 m_0 - 2\mathsf{B}_1 \mathsf{B}_2 m_1 \right)^{1/2},$$

with $m_k = M_k/|\omega|$, and we deduce Theorem 1.2. □

Proof of Lemma 1.3. Let us discuss the quantities appearing in $e(\mathbf{B}, \omega)$:

- The coefficient $m_0 m_2 - m_1^2$ corresponds to a Gram determinant, and is positive by the Cauchy–Schwarz inequality.
- The coefficient $m_0 + m_2 = \frac{1}{|\omega|} \int_\omega (\mathsf{x}_1^2 + \mathsf{x}_2^2)\, d\mathsf{x}_1\, d\mathsf{x}_2$ is the isotropic moment of order 2 in ω.
- When $(\mathsf{B}_1, \mathsf{B}_2) \neq 0$, we denote by $\Delta \subset \mathbb{R}^2$ the line borne by the projection of the magnetic field in the plane $\{\mathsf{x}_3 = 0\}$. Then the quantity

$$\int_\omega (\mathsf{B}_2 \mathsf{x}_1 - \mathsf{B}_1 \mathsf{x}_2)^2\, d\mathsf{x}_1\, d\mathsf{x}_2$$

  is the square of the L^2 norm (in ω) of the distance to Δ.

Consequently, the function $\mathbf{B} \mapsto e(\mathbf{B}, \omega)$ is a norm on $\mathbb{R}^3$. Furthermore, although the normalized moments depend on the choice of Cartesian coordinates in $\mathbb{R}^2$, the above three points show that this is not the case for the three quantities $m_0 + m_2$, $m_2 m_0 - m_1^2$ and $b_2^2 m_2 + b_1^2 m_0 - 2b_1 b_2 m_1$. We deduce that the constant $e(\mathbf{B}, \omega)$ depends only on the magnetic field and the domain and not on the choice of Cartesian coordinates. Lemma 1.3 is proved. □

3.2. Examples

In this section we apply Proposition 3.1 to particular geometries, namely discs and rectangles.

3.2.1. Circular cone. The case of a right circular cone is already considered in [5, 6], and we compare our upper bound given in Theorem 1.2 with the existing results.

For any disc ω centered at the origin, the normalized moments equal

$$m_0 = m_2 = \frac{|\omega|}{4\pi} \quad \text{and} \quad m_1 = 0,$$

so that Theorem 1.2 gives

$$E_n(\mathbf{B}, \mathcal{C}_\omega) \leq (4n-1) e(\mathbf{B}, \omega) = \frac{4n-1}{2} \sqrt{\frac{|\omega|}{\pi}} \left(\frac{\mathsf{B}_3^2}{2} + \mathsf{B}_1^2 + \mathsf{B}_2^2 \right)^{1/2}. \tag{3.4}$$

In [5, 6], the right circular cone $\mathcal{C}_\alpha^\circ$ with opening α is considered: Here ω is the disc centered at the origin with radius $\tan \frac{\alpha}{2}$. In this case, a complete asymptotic expansion is established as $\alpha \to 0$ and the first term is given by

$$\lim_{\alpha \to 0} \frac{E_n(\mathbf{B}, \mathcal{C}_\alpha^\circ)}{\alpha} = \frac{4n-1}{2^{5/2}} \sqrt{1 + \sin^2 \beta}, \tag{3.5}$$

where β is the angle between the magnetic field $\mathbf{B}$ and the axis of the cone. Let us compare with our upper bound (3.4), applied with $\mathbf{B} = (0, \sin\beta, \cos\beta)^\mathsf{T}$ and $|\omega| = \pi \tan^2 \frac{\alpha}{2}$. This provides:

$$\forall \alpha \in (0, \pi), \quad E_n(\mathbf{B}, \mathcal{C}^\circ_\alpha) \leq \frac{4n-1}{2^{3/2}} \tan\frac{\alpha}{2}\sqrt{1+\sin^2\beta}.$$

In view of (3.5), this upper bound is optimal asymptotically, as $\alpha \to 0$. Let us notice that the solution of the minimization problem (3.3) is in that case the so-called symmetric potential $\mathbf{A}'_0 = \frac{1}{2}(-\mathsf{x}_2, \mathsf{x}_1)^\mathsf{T}$ (see Proposition 3.1).

3.2.2. Rectangular cone. Let us assume that ω is the rectangle $[\ell_a, \ell_b] \times [L_a, L_b]$. The moments of order 2 can be computed explicitly:

$$m_0 = \frac{(\ell_b - \ell_a)(L_b^3 - L_a^3)}{3|\omega|} = \frac{1}{3}(L_b^2 + L_bL_a + L_a^2),$$

$$m_1 = \frac{(\ell_b^2 - \ell_a^2)(L_b^2 - L_a^2)}{4|\omega|} = \frac{1}{4}(\ell_b + \ell_a)(L_b + L_a),$$

$$m_2 = \frac{(\ell_b^3 - \ell_a^3)(L_b - L_a)}{3|\omega|} = \frac{1}{3}(\ell_b^2 + \ell_b\ell_a + \ell_a^2).$$

Let us apply Theorem 1.2 in several configurations. Note that if $\ell_a = -\ell_b$ or $L_a = -L_b$ (which means that we have a symmetry), then $m_1 = 0$ and

$$E_n(\mathbf{B}, \mathcal{C}_\omega) \leq (4n-1)\left(\mathsf{B}_3^2 \frac{m_0 m_2}{m_0 + m_2} + \mathsf{B}_1^2 m_0 + \mathsf{B}_2^2 m_2\right)^{1/2}.$$

Assuming, both $\ell_a = -\ell_b$ and $L_a = -L_b$, we obtain the following upper bound for the ground state energy for the rectangle $[-\ell, \ell] \times [-L, L]$ (for shortness, $\ell = \ell_b$ and $L = L_b$):

$$E_n(\mathbf{B}, \mathcal{C}_\omega) \leq \frac{4n-1}{\sqrt{3}}\left(\mathsf{B}_3^2 \frac{\ell^2 L^2}{\ell^2 + L^2} + \mathsf{B}_1^2 L^2 + \mathsf{B}_2^2 \ell^2\right)^{1/2}. \tag{3.6}$$

In the case of a symmetric rectangle of proportions $\ell < L = 1$, the last formula becomes

$$E_n(\mathbf{B}, \mathcal{C}_\omega) \leq \frac{4n-1}{\sqrt{3}}\left(\mathsf{B}_3^2 \frac{\ell^2}{\ell^2 + 1} + \mathsf{B}_1^2 + \mathsf{B}_2^2 \ell^2\right)^{1/2}.$$

We observe that this upper bound does not converge to 0 when $\mathsf{B}_1 \neq 0$ and ℓ tends to 0. In contrast when $\mathsf{B}_1 = 0$ there holds

$$E_n(\mathbf{B}, \mathcal{C}_\omega) \leq \frac{4n-1}{\sqrt{3}}\,\ell\left(\frac{\mathsf{B}_3^2}{\ell^2 + 1} + \mathsf{B}_2^2\right)^{1/2},$$

which tends to 0 as $\ell \to 0$. This configuration ($\mathsf{B}_1 = 0$ and $\ell \to 0$) means that $\mathbf{B}$ is almost tangent to the cone $\mathcal{C}_\omega$ in the direction where it is not sharp. This can be compared with the result (1.4) on wedges. This shows the anisotropy of the quantities appearing in our upper bounds.

For the square $[-\ell,\ell]^2$, we deduce the upper bound of the first eigenvalue

$$E_n(\mathbf{B},\mathcal{C}_\omega) \leq \frac{4n-1}{\sqrt{3}}\ell\left(\frac{\mathsf{B}_3^2}{2}+\mathsf{B}_1^2+\mathsf{B}_2^2\right)^{1/2} = \frac{4n-1}{2}\frac{\sqrt{|\omega|}}{\sqrt{3}}\left(\frac{\mathsf{B}_3^2}{2}+\mathsf{B}_1^2+\mathsf{B}_2^2\right)^{1/2}. \tag{3.7}$$

Remark 3.3. Assuming that $|\omega|$ is set, our upper bounds in the case when ω is a square or a disc can be compared, see (3.4) and (3.7). The distinct factors are

$$\frac{1}{\sqrt{\pi}} \simeq 0.5642 \quad \text{and} \quad \frac{1}{\sqrt{3}} \simeq 0.5774.$$

4. Essential spectrum for cones of small apertures with polygonal section

Here we consider the case of a family of cones parametrized by a model plane polygonal domain $\omega \subset \mathbb{R}^2$ and the scaling factor $\varepsilon > 0$. We characterize the limit of the bottom of the essential spectrum $E_{\mathrm{ess}}(\mathbf{B},\mathcal{C}_{\omega_\varepsilon})$ as $\varepsilon \to 0$, where $\mathcal{C}_{\omega_\varepsilon}$ is defined in (1.12). The main result of this section is Proposition 4.1, which is a stronger version of Proposition 1.5.

In such a situation, relations (1.10)–(1.11) take the form

$$E_{\mathrm{ess}}(\mathbf{B},\mathcal{C}_{\omega_\varepsilon}) = \mathscr{E}^*(\mathbf{B},\mathcal{C}_{\omega_\varepsilon}) = \inf_{\mathbf{p}\in\overline{\mathcal{C}_{\omega_\varepsilon}}\cap\mathbb{S}^2} E(\mathbf{B},\Pi_{\mathbf{p}}).$$

We define the bijective transformation $\mathrm{P} : \omega \times \mathbb{R}_+ \to \mathcal{C}_\omega$ by

$$\mathrm{P}(\mathbf{x}',t) = t\,\frac{(\mathbf{x}',1)}{\|(\mathbf{x}',1)\|}, \qquad \forall(\mathbf{x}',t)\in\omega\times\mathbb{R}_+. \tag{4.1}$$

Notice that $\mathbf{x}' \mapsto \mathrm{P}(\mathbf{x}',1)$ defines a bijection from $\mathbb{R}^2$ onto the upper half-sphere $\mathbb{S}^2_+ := \{\mathbf{p}\in\mathbb{S}^2,\ \mathsf{p}_3 > 0\}$, and that for all $\varepsilon > 0$, $\mathrm{P}(\varepsilon\omega,1)$ is an open set of $\mathbb{S}^2_+$ and coincides with $\mathcal{C}_{\omega_\varepsilon}\cap\mathbb{S}^2$.

If $\mathbf{p}$ is a vertex of $\mathcal{C}_{\omega_\varepsilon}\cap\mathbb{S}^2$, then $\mathbf{x}' = \mathrm{P}(\cdot,1)^{-1}(\mathbf{p})$ is still a vertex of ω_ε, but its opening angle is not the same as for $\mathbf{p}$, in particular the tangent cones $\Pi_{\mathbf{p}}$ and $\widehat{\Pi}_{\mathbf{x}'}$ are both wedges, but they cannot be deduced each one from another by a rotation, and in general the ground state energies on these two domains are different.

The following proposition estimates the difference between the ground state energies as $\varepsilon \to 0$:

Proposition 4.1. *There exist positive constants ε_0 and $C(\omega)$ depending only on ω such that*

$$\forall\varepsilon\in(0,\varepsilon_0), \qquad |\mathscr{E}^*(\mathbf{B},\mathcal{C}_{\omega_\varepsilon}) - \mathscr{E}(\mathbf{B},\widehat{\omega})| \leq C(\omega)\,\varepsilon^{1/3}. \tag{4.2}$$

In particular, $\lim_{\varepsilon\to 0}\mathscr{E}^*(\mathbf{B},\mathcal{C}_{\omega_\varepsilon}) = \mathscr{E}(\mathbf{B},\widehat{\omega})$.

Proof. Recall that the transformation P is defined in (4.1). Denote by $\mathbf{0}$ the origin in the plane $\mathbb{R}^2$. The differential $\mathrm{d}_{(\mathbf{0},1)}\mathrm{P}$ of P at the point $(\mathbf{0},1)$ is the identity $\mathbb{I}$. So there exist positive constants C and ε_0 such that for all $\varepsilon\in(0,\varepsilon_0)$,

$$\forall\mathbf{x}'\in\overline{\omega_\varepsilon}, \quad \|\,\mathrm{d}_{(\mathbf{x}',1)}\mathrm{P} - \mathbb{I}\,\| \leq C\varepsilon. \tag{4.3}$$

Define N_ε the scaling of ratio ε around the plane $t=1$:

$$\mathrm{N}_\varepsilon : (\mathsf{x}_1, \mathsf{x}_2, t) \longmapsto (\varepsilon \mathsf{x}_1, \varepsilon \mathsf{x}_2, 1+\varepsilon(t-1)). \tag{4.4}$$

The scaling N_ε transforms a neighborhood of $\overline{\varpi}\times\{1\}$ into a neighborhood of $\varepsilon\overline{\varpi}\times\{1\}$. Then the composed application $\mathrm{P}\circ\mathrm{N}_\varepsilon$ is a diffeomorphism from a neighborhood of $\overline{\varpi}\times\{1\}$ onto a neighborhood of $\mathcal{C}_{\omega_\varepsilon}\cap\mathbb{S}^2$.

Let us pick a point $\mathbf{x}'$ in the closure of the polygonal domain ω. By definition of polygonal domains, there exists a local diffeomorphism J that sends a neighborhood of $\mathbf{x}'$ in $\overline{\varpi}$ onto a neighborhood of $\mathbf{0}$ of the tangent plane sector (in broad sense) $\Pi_{\mathbf{x}'}$. The differential $\mathrm{d}_{\mathbf{x}'}\mathrm{J}$ equals $\mathbb{I}$ by construction. Then $\widehat{\mathrm{J}} := \mathrm{J}\otimes\mathbb{I}_3$ realizes a local diffeomorphism that sends a neighborhood of $\mathbf{x}:=(\mathbf{x}',1)$ in $\overline{\widehat{\omega}}$ onto a neighborhood of $\mathbf{0}$ of the tangent cone $\widehat{\Pi}_{\mathbf{x}} := \Pi_{\mathbf{x}'}\times\mathbb{R}$.

We set $\mathbf{p}_\varepsilon := \mathrm{P}\circ\mathrm{N}_\varepsilon(\mathbf{x})$. For any $\varepsilon\in(0,\varepsilon_0)$, the composed application

$$\widehat{\mathrm{J}}\circ(\mathrm{P}\circ\mathrm{N}_\varepsilon)^{-1}$$

is a local diffeomorphism that sends a neighborhood of the point $\mathbf{p}_\varepsilon$ in $\overline{\mathcal{C}}_{\varepsilon\omega}$ onto a neighborhood of $\mathbf{0}$ of the cone $\widehat{\Pi}_{\mathbf{x}}$. Let D_ε be the differential at $\mathbf{0}$ of the inverse of the map $\widehat{\mathrm{J}}\circ(\mathrm{P}\circ\mathrm{N}_\varepsilon)^{-1}$. Then, by construction, the modified map

$$\mathrm{D}_\varepsilon\circ\widehat{\mathrm{J}}\circ(\mathrm{P}\circ\mathrm{N}_\varepsilon)^{-1}$$

is such that its differential at the point $\mathbf{p}_\varepsilon$ is the identity $\mathbb{I}$. Therefore this modified map is a local diffeomorphism that sends a neighborhood of the point $\mathbf{p}_\varepsilon$ in $\overline{\mathcal{C}_{\omega_\varepsilon}}$ onto a neighborhood of $\mathbf{0}$ in the *tangent* cone $\Pi_{\mathbf{p}_\varepsilon}$.

We deduce that D_ε is a linear isomorphism between the two cones of interest

$$\mathrm{D}_\varepsilon : \widehat{\Pi}_{\mathbf{x}} \longmapsto \Pi_{\mathbf{p}_\varepsilon}\,.$$

We calculate:

$$\mathrm{D}_\varepsilon = \mathrm{d}_{\mathbf{0}}(\mathrm{P}\circ\mathrm{N}_\varepsilon\circ\widehat{\mathrm{J}}^{-1}) = \mathrm{d}_{\mathbf{p}_\varepsilon}\mathrm{P}\circ\mathrm{d}_{\mathbf{x}}\mathrm{N}_\varepsilon\circ\mathrm{d}_0\widehat{\mathrm{J}}^{-1}\,.$$

But $\mathrm{d}_{\mathbf{0}}\widehat{\mathrm{J}}^{-1}=\mathbb{I}$ and $\mathrm{d}_{\mathbf{x}}\mathrm{N}_\varepsilon=\varepsilon\,\mathbb{I}$. So we have obtained that $\varepsilon\,\mathrm{d}_{\mathbf{p}_\varepsilon}\mathrm{P}$ is an isomorphism between the two cones of interest. By homogeneity $\mathrm{d}_{\mathbf{p}_\varepsilon}\mathrm{P}$ is also an isomorphism between the same sets. Thanks to (4.3) we have obtained that

Lemma 4.2. *Let* $\mathbf{x}'\in\overline{\varpi}$, $\mathbf{x}=(\mathbf{x}',1)$ *and* $\mathbf{p}_\varepsilon=\mathrm{P}\circ\mathrm{N}_\varepsilon(\mathbf{x})$. *Then the linear map* $\mathrm{L}_{\mathbf{x},\varepsilon}:=\mathrm{d}_{\mathbf{p}_\varepsilon}\mathrm{P}$ *is an isomorphism between* $\widehat{\Pi}_{\mathbf{x}}$ *and* $\Pi_{\mathbf{p}_\varepsilon}$, *that satisfies*

$$\|\mathrm{L}_{\mathbf{x},\varepsilon}-\mathbb{I}\,\|\le C\varepsilon, \tag{4.5}$$

where C depends neither on $\mathbf{x}'$ *nor on* ε *and with* $\mathrm{P},\mathrm{N}_\varepsilon$ *defined in* (4.1), (4.4).

Therefore

$$E(\mathbf{B},\widehat{\Pi}_{\mathbf{x}})-E(\mathbf{B},\Pi_{\mathbf{p}_\varepsilon}) = E(\mathbf{B},\widehat{\Pi}_{\mathbf{x}})-E(\mathbf{B},\mathrm{L}_{\mathbf{x},\varepsilon}(\widehat{\Pi}_{\mathbf{x}})). \tag{4.6}$$

Relying on (4.5), we are going to estimate the right-hand side of (4.6) depending on the position of $\mathbf{x}'\in\overline{\varpi}$:

(a) $\mathbf{x}'$ is inside ω. Then $\widehat{\Pi}_{\mathbf{x}}$ is the full space $\mathbb{R}^3$, just like $\mathrm{L}_{\mathbf{x},\varepsilon}(\widehat{\Pi}_{\mathbf{x}})$. So $E(\mathbf{B},\widehat{\Pi}_{\mathbf{x}})$ coincides with $E(\mathbf{B},\mathrm{L}_{\mathbf{x},\varepsilon}(\widehat{\Pi}_{\mathbf{x}}))$ in this case.

(b) $\mathbf{x}'$ belongs to a side of ω. Then $\widehat{\Pi}_{\mathbf{x}}$ and $\mathrm{L}_{\mathbf{x},\varepsilon}(\widehat{\Pi}_{\mathbf{x}})$ are half-spaces. The lowest energy $E(\mathbf{B},\Pi)$ when Π is a half-space is determined by the $\mathscr{C}^1$ function σ acting on the unsigned angle $\theta \in [0,\frac{\pi}{2}]$ between $\mathbf{B}$ and $\partial\Pi$. If $\theta_{\mathbf{x}}$, $\theta_{\mathbf{x},\varepsilon}$ denote the angle between $\mathbf{B}$ and $\partial\widehat{\Pi}_{\mathbf{x}}$, $\partial\mathrm{L}_{\mathbf{x},\varepsilon}(\widehat{\Pi}_{\mathbf{x},\varepsilon})$, respectively, then for a constant C depending on ω:

$$|\theta_{\mathbf{x}} - \theta_{\mathbf{x},\varepsilon}| \leq C\varepsilon \quad \text{and} \quad |\sigma(\theta_{\mathbf{x}}) - \sigma(\theta_{\mathbf{x},\varepsilon})| \leq C\varepsilon. \tag{4.7}$$

(c) $\mathbf{x}'$ is a corner of ω. Then $\widehat{\Pi}_{\mathbf{x}}$ and $\mathrm{L}_{\mathbf{x},\varepsilon}(\widehat{\Pi}_{\mathbf{x}})$ are wedges of opening $\alpha_{\mathbf{x}}$ and $\alpha_{\mathbf{x},\varepsilon}$ with $|\alpha_{\mathbf{x}} - \alpha_{\mathbf{x},\varepsilon}| \leq C\varepsilon$. Moreover there exist rotations $\mathrm{R}_{\mathbf{x}}$ and $\mathrm{R}_{\mathbf{x},\varepsilon}$ that transform $\widehat{\Pi}_{\mathbf{x}}$ and $\mathrm{L}_{\mathbf{x},\varepsilon}(\widehat{\Pi}_{\mathbf{x}})$ into the canonical wedges $\mathcal{W}_{\alpha_{\mathbf{x}}}$ and $\mathcal{W}_{\alpha_{\mathbf{x},\varepsilon}}$ and there holds $\|\mathrm{R}_{\mathbf{x},\varepsilon} - \mathrm{R}_{\mathbf{x}}\| \leq C\varepsilon$. Since

$$E(\mathbf{B},\widehat{\Pi}_{\mathbf{x}}) = E(\mathrm{R}_{\mathbf{x}}^{-1}\mathbf{B},\mathcal{W}_{\alpha_{\mathbf{x}}}) \quad \text{and} \quad E(\mathbf{B},\mathrm{L}_{\mathbf{x},\varepsilon}(\widehat{\Pi}_{\mathbf{x}})) = E(\mathrm{R}_{\mathbf{x},\varepsilon}^{-1}\mathbf{B},\mathcal{W}_{\alpha_{\mathbf{x},\varepsilon}}),$$

we deduce from [19, Section 4.4]

$$|E(\mathbf{B},\widehat{\Pi}_{\mathbf{x}}) - E(\mathbf{B},\mathrm{L}_{\mathbf{x},\varepsilon}(\widehat{\Pi}_{\mathbf{x}}))| \leq C\varepsilon^{1/3}.$$

Taking the infimum over $\mathbf{x} \in \overline{\omega}\times\{1\}$, we deduce the (4.2). As stated in [4, Corollary 8.5], there holds $\mathscr{E}(\mathbf{B},\widehat{\omega}) > 0$. Therefore we deduce Proposition 4.1. □

5. Application to corner concentration

In this section, we discuss the link between (1.16) and (1.17), and we then prove Proposition 1.8.

We first prove that condition (1.17) implies condition (1.16). If (1.17) holds, there exists a vertex $\mathbf{v}$ such that $\mathscr{E}(\mathbf{B},\Omega) = E(\mathbf{B},\Pi_{\mathbf{v}})$. By [4, Theorem 6.6], the essential spectrum of $H(\mathbf{A},\Pi_{\mathbf{v}})$ is given by

$$\mathscr{E}^*(\mathbf{B},\Pi_{\mathbf{v}}) := \inf_{\mathbf{p}\,\in\,\overline{\Pi_{\mathbf{v}}}\cap\mathbb{S}^2} E(\mathbf{B},\Pi_{\mathbf{p}}).$$

But for each $\mathbf{p} \in \overline{\Pi_{\mathbf{v}}}\cap\mathbb{S}^2$, the cone $\Pi_{\mathbf{v}}$ is the limit of tangent cones $\Pi_{\mathbf{x}}$ with points $\mathbf{x} \in \overline{\Omega}\setminus\mathfrak{V}$ converging to $\mathbf{v}$. The continuity of the ground energy then implies that

$$E(\mathbf{B},\Pi_{\mathbf{p}}) \geq \inf_{\mathbf{x}\in\overline{\Omega}\setminus\mathfrak{V}} E(\mathbf{B},\Pi_{\mathbf{x}}).$$

We deduce

$$\mathscr{E}^*(\mathbf{B},\Pi_{\mathbf{v}}) \geq \inf_{\mathbf{x}\in\overline{\Omega}\setminus\mathfrak{V}} E(\mathbf{B},\Pi_{\mathbf{x}}).$$

Hence condition (1.16) holds.

Proof of point a) *of Proposition* 1.8. By condition i), and as a consequence of (1.7) and (1.13), there holds

$$E(\mathbf{B},\Pi_{\mathbf{v}(\varepsilon)}) \leq 3\varepsilon\, e(\mathbf{B},\omega). \tag{5.1}$$

Let us bound $\inf_{\mathbf{x}\in\overline{\Omega}\setminus\mathfrak{V}} E(\mathbf{B},\Pi_{\mathbf{x}})$ from below. Let $\mathbf{x} \in \overline{\Omega}\setminus\mathfrak{V}$.

1. If $\mathbf{x}$ is an interior point, then $E(\mathbf{B},\Pi_{\mathbf{x}}) = E(\mathbf{B},\mathbb{R}^3) = \|\mathbf{B}\|$.
2. If $\mathbf{x}$ belongs to a face, $\Pi_{\mathbf{x}}$ is a half-space and $E(\mathbf{B},\Pi_{\mathbf{x}}) \geq \Theta_0\|\mathbf{B}\| > \frac{1}{2}\|\mathbf{B}\|$.

3. Since x is not a vertex, it remains the case when x belongs to an edge of Ω, and then Π_{x} is a wedge. Let α_{x} denote its opening. Then $E(\mathbf{B}, \Pi_{\mathsf{x}}) = E(\mathbf{B}_{\mathsf{x}}, \mathcal{W}_{\alpha_{\mathsf{x}}})$ where $\mathbf{B}_{\mathsf{x}}$ is deduced from $\mathbf{B}$ by a suitable rotation. At this point we use the continuity result of [19, Theorem 4.5] for $(\mathbf{B}, \alpha) \mapsto E(\mathbf{B}, \alpha)$ with respect to $\alpha \in (0, 2\pi)$ and $\mathbf{B} \in \mathbb{S}^2$, which yields
$$\min_{\beta_0 \le \alpha \le 2\pi - \beta_0,\ \|\mathbf{B}\|=1} E(\mathbf{B}, \mathcal{W}_\alpha) =: c(\beta_0) > 0, \tag{5.2}$$
where the diamagnetic inequality has been used to get the positivity. We deduce by homogeneity $E(\mathbf{B}, \Pi_{\mathsf{x}}) \ge c(\beta_0)\|\mathbf{B}\|$.

Finally
$$\inf_{\mathsf{x} \in \overline{\Omega} \setminus \mathfrak{V}} E(\mathbf{B}, \Pi_{\mathsf{x}}) \ge \min\{c(\beta_0), \tfrac{1}{2}\}\|\mathbf{B}\|.$$

Combined with the previous upper bound (5.1) at the vertex $\mathbf{v}(\varepsilon)$, this estimate yields that condition (1.17) is satisfied for ε small enough, hence point a) of Proposition 1.8.

Proof of point b) *of Proposition* 1.8. Let us define
$$\Omega(\varepsilon) = \mathcal{C}_{\omega_\varepsilon} \cap \{\mathsf{x}_3 < 1\}.$$

By construction, we only have to check (1.19). The edges of $\Omega(\varepsilon)$ can be classified in two sets:

1. The edges contained in those of $\mathcal{C}_{\omega_\varepsilon}$. We have proved in Section 4 that their opening converge to the opening angles of ω as $\varepsilon \to 0$.
2. The edges contained in the plane $\{\mathsf{x}_3 = 1\}$. Their openings tend to $\frac{\pi}{2}$ as $\varepsilon \to 0$.

Hence (1.19).

6. Analogies with the Robin Laplacian

We describe here some similarities of the Neumann magnetic Laplacian with the Robin Laplacian on corner domains. For a real parameter γ, this last operator acts as the Laplacian on functions satisfying the mixed boundary condition $\partial_n u - \gamma u = 0$ where ∂_n is the outward normal and γ is a real parameter. The associated quadratic form is
$$u \mapsto \int_\Omega |\nabla u(x)|^2 \,\mathrm{d}x - \gamma \int_{\partial\Omega} |u(s)|^2 \,\mathrm{d}s, \quad u \in \mathrm{H}^1(\Omega).$$

Since the study initiated in [13], many works have been done in order to understand the asymptotics of the eigenpairs of this operator in the limit $\gamma \to +\infty$. It occurs that in this regime, the first eigenvalue $\lambda_\gamma^{\mathsf{Rob}}(\Omega)$ of this Robin Laplacian shares numerous common features with those of the magnetic Laplacian in the semi-classical limit. Levitin and Parnovski prove that for a corner domain Ω satisfying a uniform interior cone condition, there holds (see [14, Theorem 3.2])

$$\lambda_\gamma^{\mathsf{Rob}}(\Omega) \underset{\gamma\to+\infty}{\sim} \gamma^2 \inf_{\mathbf{x}\in\partial\Omega} E^{\mathsf{Rob}}(\Pi_{\mathbf{x}}), \tag{6.1}$$

where, as before, $E^{\mathsf{Rob}}(\Pi_{\mathbf{x}})$ is the ground state energy of the model operator ($\gamma = 1$) on the tangent cone $\Pi_{\mathbf{x}}$ at $\mathbf{x}$. In fact, $E^{\mathsf{Rob}}(\Pi_{\mathbf{x}}) < 0$ for any boundary point $\mathbf{x}$. This result leads to the same problematics as ours: compare the ground state energies of model operators on various tangent cones. When $\Pi_{\mathbf{x}}$ is either a half-space or a wedge, $E^{\mathsf{Rob}}(\Pi_{\mathbf{x}})$ is explicit:

$$E^{\mathsf{Rob}}(\mathbb{R}^3_+) = -1 \quad \text{and} \quad E^{\mathsf{Rob}}(\mathcal{W}_\alpha) = \begin{cases} -\sin^{-2}(\frac{\alpha}{2}) & \text{if} \ \ \alpha \in (0,\pi] \\ -1 & \text{if} \ \ \alpha \in [\pi, 2\pi). \end{cases} \tag{6.2}$$

This shows, in some sense, that the Robin Laplacian is simpler for these cones. We notice that $E^{\mathsf{Rob}}(\mathcal{W}_\alpha) \to -\infty$ as $\alpha \to 0$. This fact should be compared to (1.4). The general idea behind this is an analogy between the degeneracy of the ground state energies, as follows: Whereas the ground energy (always positive) is going to 0 for the magnetic Laplacian on sharp cones, the ground energy (always finite) of the Robin Laplacian goes to $-\infty$, as we shall explain below.

However, for cones of higher dimensions, no explicit expression like (6.2) is known for $E^{\mathsf{Rob}}(\Pi_{\mathbf{x}})$. In [14, Section 5], a two-sided estimate is given for convex cones of dimension ≥ 3. The idea for this estimate is quite similar to our strategy: Given a suitable reference axis $\{\mathsf{x}_3 > 0\}$ intersecting $\Pi \cap \mathbb{S}^2$ at a point denoted by θ, one defines the plane P tangent to $\mathbb{S}^2$ at θ, so that the intersection $P \cap \Pi$ defines a section ω for which the cone Π coincides with $\mathcal{C}_\omega$ given by (1.5). Using polar coordinates $(\rho, \phi) \in \mathbb{R}^+ \times \mathbb{S}^1$ in the plane P centered at θ, one parametrizes the boundary of ω by a function b through the relation $\rho = b(\phi)$. Then[1], [14, Theorem 5.1] provides the upper bound

$$E^{\mathsf{Rob}}(\Pi) \leq -\left(\frac{\int_{\mathbb{S}^1} \sigma(\phi)\, b(\phi)^2 \,\mathrm{d}\phi}{\int_{\mathbb{S}^1} b(\phi)^2 \,\mathrm{d}\phi}\right)^2 \quad \text{with} \quad \sigma(\phi) = \sqrt{1 + b(\phi)^{-2} + b'(\phi)^2 b(\phi)^{-4}}. \tag{6.3}$$

Note that this estimate depends on the choice of the reference coordinate x_3, exactly as in our case, see Remark 1.4, and can be optimized by taking the infimum on θ.

Estimate (6.3) shows in particular that for our sharp cones $\mathcal{C}_{\omega_\varepsilon}$, the energy $E^{\mathsf{Rob}}(\mathcal{C}_{\omega_\varepsilon})$ goes to $-\infty$ like $-\varepsilon^{-2}$ as $\varepsilon \to 0$. This property is the analog of our upper bounds (1.7)-(1.13). We expect that an analog of our formula (1.11) is valid, implying that there exists a finite limit for the bottom of the essential spectrum of the model Robin Laplacians defined on $\mathcal{C}_{\omega_\varepsilon}$, as $\varepsilon \to 0$. This would provide similar conclusions for Robin problem and for the magnetic Laplacian.

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[1] In [14, Theorem 5.1], the quantity $-E^{\mathsf{Rob}}(\Pi)$ is estimated, so that the upper bound presented here, corresponds to the lower bound of the paper *loc. cit.*

Appendix: Tangent cones and corner domains

Following [7, Section 2] (see also [4, Section 1]), we recall the definition of corner domains. We call a *cone* any open subset Π of $\mathbb{R}^n$ satisfying

$$\forall \rho > 0 \ \text{ and } \ \mathsf{x} \in \Pi, \quad \rho\mathsf{x} \in \Pi,$$

and the *section* of the cone Π is its subset $\Pi \cap \mathbb{S}^{n-1}$. Note that $\mathbb{S}^0 = \{-1, 1\}$.

Definition A.1 (Tangent cone)**.** Let Ω be an open subset of $M = \mathbb{R}^n$ or $\mathbb{S}^n$. Let $\mathsf{x}_0 \in \overline{\Omega}$. The cone Π_{x_0} is said to be *tangent to* Ω at x_0 if there exists a local $\mathscr{C}^\infty$ diffeomorphism $\mathrm{U}^{\mathsf{x}_0}$ which maps a neighborhood $\mathcal{U}_{\mathsf{x}_0}$ of x_0 in M onto a neighborhood $\mathcal{V}_{\mathsf{x}_0}$ of $\mathbf{0}$ in $\mathbb{R}^n$ and such that

$$\mathrm{U}^{\mathsf{x}_0}(\mathsf{x}_0) = \mathbf{0}, \quad \mathrm{U}^{\mathsf{x}_0}(\mathcal{U}_{\mathsf{x}_0} \cap \Omega) = \mathcal{V}_{\mathsf{x}_0} \cap \Pi_{\mathsf{x}_0} \quad \text{and} \quad \mathrm{U}^{\mathsf{x}_0}(\mathcal{U}_{\mathsf{x}_0} \cap \partial\Omega) = \mathcal{V}_{\mathsf{x}_0} \cap \partial\Pi_{\mathsf{x}_0}.$$

Definition A.2 (Class of corner domains)**.** For $M = \mathbb{R}^n$ or $\mathbb{S}^n$, the classes of corner domains $\mathfrak{D}(M)$ and tangent cones $\mathfrak{P}_n$ are defined as follows:

Initialization: $\mathfrak{P}_0$ has one element, $\{0\}$. $\mathfrak{D}(\mathbb{S}^0)$ is formed by all subsets of $\mathbb{S}^0$.

Recurrence: For $n \geq 1$,

(1) $\Pi \in \mathfrak{P}_n$ if and only if the section of Π belongs to $\mathfrak{D}(\mathbb{S}^{n-1})$,

(2) $\Omega \in \mathfrak{D}(M)$ if and only if for any $\mathsf{x}_0 \in \overline{\Omega}$, there exists a tangent cone $\Pi_{\mathsf{x}_0} \in \mathfrak{P}_n$ to Ω at x_0.

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Spectral Clusters for Magnetic Exterior Problems

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Abstract. Let $H_0 = (i\nabla - A)^2$ be the Schrödinger operator with constant magnetic field in $\mathbb{R}^d$, $d = 2, 3$ and $K \subset \mathbb{R}^d$ be a compact domain with smooth boundary. We consider the Dirichlet (resp. Neumann, resp. Robin) realization of $(i\nabla - A)^2$ on $\Omega := \mathbb{R}^d \setminus K$. First, in the case $d = 2$, we recall the known results concerning eigenvalue clusters for these exterior problems. Then, in dimension 3, after a review on the previous results for potential perturbations, we study the resonances for the obstacle problems. We establish the existence of resonance free sectors near the Landau level and study a resonance counting function. Consequently we obtain the accumulation of resonances at the Landau levels and in some cases the discretness of the set of the embedded eigenvalues.

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1. Introduction

We consider, in $\mathbb{R}^3$, a constant magnetic field of strength $b > 0$, pointing at the x_3-direction, $B = (0, 0, b)$. For an associated magnetic potential $A = (A_1, A_2, A_3) = (-b\frac{x_2}{2}, b\frac{x_1}{2}, 0)$ let us introduce the magnetic derivatives:

$$\nabla_j^A := \nabla_{x_j} - iA_j; \quad j = 1, 2, 3$$

and the magnetic Schrödinger operators in $\mathbb{R}^d$, $d = 2, 3$:

$$-\left(\nabla^A\right)^2 := -\sum_{j=1}^{d} \left(\nabla_j^A\right)^2 = \begin{cases} \left(D_1 + \frac{b}{2}x_2\right)^2 + \left(D_2 - \frac{b}{2}x_1\right)^2 & \text{if} \quad d = 2, \\ \left(D_1 + \frac{b}{2}x_2\right)^2 + \left(D_2 - \frac{b}{2}x_1\right)^2 + D_3^2 & \text{if} \quad d = 3 \end{cases} \tag{1.1}$$

where $D_j := -i\frac{\partial}{\partial x_j}$ is the symmetric partial derivative.

The aim of this paper is to give spectral properties of these operators in presence of an obstacle. Let $K \subset \mathbb{R}^d$, $d = 2, 3$, be a compact domain with smooth boundary Σ and let $\Omega := \mathbb{R}^d \setminus K$. We denote by ν the unit outward normal vector of the boundary Σ and by $\partial_\nu^A := \nabla^A \cdot \nu$ the magnetic normal derivative. For γ a smooth real-valued function on Σ, we introduce the operator

$$\partial_\Sigma^{A,\gamma} := \nabla^A \cdot \nu + \gamma$$

and the quadratic form

$$Q_\Omega^\gamma(u) = \int_\Omega \left|\nabla^A u\right|^2 dx + \int_\Sigma \gamma |u|^2 d\sigma. \tag{1.2}$$

Then, we define the Robin, the Neumann and the Dirichlet realizations of $-\left(\nabla^A\right)^2$ on Ω:

- H_Ω^γ, the Robin operator, is the self-adjoint operator associated with the closure of the quadratic form Q_Ω^γ originally defined in the magnetic Sobolev space $H_A^1(\Omega) := \left\{u \in L^2(\Omega) : \nabla^A u \in L^2(\Omega)\right\}$.
- H_Ω^0, the Neumann operator, corresponds to the Robin operator with $\gamma = 0$.
- H_Ω^∞, the Dirichlet operator, is the self-adjoint operator associated with the closure of the quadratic form Q_Ω^0 originally defined on $C_0^\infty(\Omega)$.

These operators will be considered as perturbations of the reference operator H_0, the self-adjoint operator associated with the closure of the quadratic form on $\mathbb{R}^d$, $Q_{\mathbb{R}^d}^0$ originally defined on $C_0^\infty(\mathbb{R}^d)$, $d = 2, 3$.

Thus, the operator H_Ω^γ is defined by

$$\begin{cases} H_\Omega^\gamma u = -\left(\nabla^A\right)^2 u, \quad u \in \mathrm{Dom}\left(H_\Omega^\gamma\right), \\ \mathrm{Dom}\left(H_\Omega^\gamma\right) := \left\{u \in L^2(\Omega) : \left(\nabla^A\right)^k u \in L^2(\Omega),\ k = 1, 2\ :\ \partial_\Sigma^{A,\gamma} u = 0 \text{ on } \Sigma\right\}, \end{cases} \tag{1.3}$$

the operator H_Ω^∞ by

$$\begin{cases} H_\Omega^\infty u = -\left(\nabla^A\right)^2 u, \quad u \in \mathrm{Dom}\left(H_\Omega^\infty\right), \\ \mathrm{Dom}\left(H_\Omega^\infty\right) := \left\{u \in L^2(\Omega) : \left(\nabla^A\right)^k u \in L^2(\Omega),\ k = 1, 2\ :\ u = 0 \text{ on } \Sigma\right\}, \end{cases} \tag{1.4}$$

and H_0 satisfies

$$\begin{cases} H_0 u = -\left(\nabla^A\right)^2 u, \quad u \in \mathrm{Dom}\left(H_0\right) = H_A^2(\mathbb{R}^d), \\ H_A^2(\mathbb{R}^d) := \left\{u \in L^2(\mathbb{R}^d) : \left(\nabla^A\right)^k u \in L^2(\mathbb{R}^d),\ k = 1, 2\right\}. \end{cases} \tag{1.5}$$

Let us mention that magnetic boundary problems appear in the Ginzburg–Landau theory of superconductors, in the theory of Bose–Einstein condensates, and in the study of edge states in Quantum Mechanics (see for instance [9], [15], [1], [12],...).

This paper is a review of known results concerning the spectrum of the above operators. The 2D cases were studied by Pushnitski–Rozenblum [21] for the Dirichlet problem, by Persson Sundqvist [20] for the Neumann problem and by Goffeng–Kachmar–Persson Sundqvist [13] for the Robin boundary condition. The 3D cases are contained in the recent work of the authors [8]. These results are closely related to previous works concerning perturbations of H_0 by potentials V of definite sign, $H = H_0 + V$, with V compactly supported (see [22], [23], [19], [10] in the 2D case and [6], [11], [4], [5] in the 3D case).

As we will see, an important difference between the 2D and the 3D case is the spectral structure of H_0. In dimension 2, the so-called *Landau Hamiltonian*, H_0, admits a pure point spectrum (and the same holds for the relatively compact perburbations), while in dimension 3, the spectrum of H_0 is absolutely continuous. Thus, in dimension 3, the spectral properties of relatively compact perturbations of H_0 are analysed with the study of the Spectral Shift Function or of the resonances.

2. Results in the 2-dimensional case

In $\mathbb{R}^2$, the reference operator H_0 is the Landau Hamiltonian:

$$H_0 = H_{\text{Landau}} := \Big(D_1 + \frac{b}{2}x_2\Big)^2 + \Big(D_2 - \frac{b}{2}x_1\Big)^2. \tag{2.1}$$

Its spectrum consists of the so-called Landau levels $\Lambda_q = (2q+1)b$, $q \in \mathbb{N} := \{0, 1, 2, \dots\}$, and $\dim \operatorname{Ker}(H_{\text{Landau}} - \Lambda_q) = \infty$ (see for instance [2]), that is the spectrum and the essential spectrum of H_0 coincide with the point spectrum:

$$\sigma(H_0) = \sigma_{\text{ess}}(H_0) = \sigma_p(H_0) = \{\Lambda_q;\ q \geq 0\}.$$

For the exterior problem, Weyl's theorem on the invariance of the essential spectrum under compact perturbation allows us to prove (see [15], [21], [16], [20], [13]) that:

$$\sigma_{\text{ess}}(H_\Omega^\infty) = \sigma_{\text{ess}}(H_\Omega^\gamma) = \sigma_{\text{ess}}(H_0) = \{\Lambda_q;\ q \geq 0\}.$$

Thus, the spectrum of the operators H_Ω^∞ and H_Ω^γ is discrete outside the Landau levels and the discrete eigenvalues can only accumulate to the Landau levels.

Finally, if the obstacle K has a non-empty interior, for the Dirichlet problem, Pushnitski–Rozenblum [21] proves that below (resp. above) each Landau level, H_Ω^∞ has a finite number of eigenvalues (resp. infinitely many eigenvalues). On the contrary, for H_Ω^γ Persson Sundqvist [20] and Goffeng–Kachmar–Persson Sundqvist [13] proves that the eigenvalues accumulate only below each Landau level. More precisely, if for an operator H and $q \in \mathbb{N}$ fixed, we introduce the counting function:

$$\mathcal{N}_\pm(H, r) := \#\{\text{eig.}(H) \in \Lambda_q \pm (r, r_0)\}, \qquad 0 < r < r_0 < 2b,$$

we have:

Theorem 2.1 ([21], [20] and [13]). *Suppose the obstacle K has a non-empty interior. Then as $r \searrow 0$, the counting functions of the eigenvalues of H_Ω^∞ and of H_Ω^γ on the* *right, and on the left of the Landau levels satisfy:*

$$\mathcal{N}_-(H_\Omega^\infty, r) = O(1), \qquad \mathcal{N}_+(H_\Omega^\infty, r) \sim |\ln r| \, (\ln|\ln r|)^{-1},$$
$$\mathcal{N}_-(H_\Omega^\gamma, r) \sim |\ln r| \, (\ln|\ln r|)^{-1}, \quad \mathcal{N}_+(H_\Omega^\gamma, r) = O(1).$$

Let us mention that the above theorem is a consequence of more accurate results of the cited works where the asymptotic behavior of each discrete eigenvalue is studied. These results are closely related to previous results of Raikov–Warzel [23], Melgaard–Rozenblum [19] and Filonov–Pushnitski [10] where the perturbation of H_0 by potentials are considered. In particular, for $\mathbb{1}_K$, the characteristic function of K, these results state that, as $r \searrow 0$ one has:

$$\mathcal{N}_-(H_0 + \mathbb{1}_K, r) = O(1), \qquad \mathcal{N}_+(H_0 + \mathbb{1}_K, r) \sim |\ln r| \, (\ln|\ln r|)^{-1},$$
$$\mathcal{N}_-(H_0 - \mathbb{1}_K, r) \sim |\ln r| \, (\ln|\ln r|)^{-1}, \quad \mathcal{N}_+(H_0 - \mathbb{1}_K, r) = O(1).$$

Thus the distribution of the eigenvalues of H_Ω^∞ (resp. of H_Ω^γ) follows the same law as this of the eigenvalues of $H_0 + \mathbb{1}_K$ (resp. of $H_0 - \mathbb{1}_K$). Since the main term of the above asymptotics is independent of K, the characteristic function of K can be replaced by any compactly supported function with support having a non-empty interior. However the more refined asymptotics mentioned above for the obstacle problems and for the potential perturbation coincide only if the support of the perturbed potential is K (or is a set with the same capacity) because these asymptotics involve the capacity of the set K (see [19], [10], [21], [20] and [13]).

3. Perturbation of H_0 in dimension 3

3.1. Spectral properties

In the three-dimensional case, the reference operator H_0 is related to the Landau Hamiltonian (defined by (2.1)). By identifying $L^2(\mathbb{R}^3)$ with $L^2(\mathbb{R}^2_{(x_1,x_2)}) \otimes L^2(\mathbb{R}_{x_3})$, we have:

$$H_0 = H_{\text{Landau}} \otimes I_3 + I_\perp \otimes D_3^2 \tag{3.1}$$

with I_3 and $I_\perp$ being the identity operators in $L^2(\mathbb{R}_{x_3})$ and $L^2(\mathbb{R}^2_{(x_1,x_2)})$ respectively. Consequently, since the spectrum of H_{Landau} consists of the Landau levels, and $\sigma(D_3^2) = \sigma_{\text{ac}}(D_3^2) = [0 + \infty)$, then

$$\sigma(H_0) = \sigma_{\text{ac}}(H_0) = \cup_{q\geq 0}\Big(\Lambda_q + [0, +\infty)\Big) = [b, +\infty),$$

and the Landau levels play the role of thresholds in the spectrum of H_0. As in the two-dimensional case, for the exterior problems, Weyl's theorem allows us to prove (see [16]) that

$$\sigma_{\text{ess}}(H_\Omega^\infty) = \sigma_{\text{ess}}(H_\Omega^\gamma) = \sigma_{\text{ess}}(H_0) = \sigma(H_0) = [b, +\infty).$$

In this case, due to the presence of continuous spectrum on the semi-axis $[b, +\infty)$, the clusters phenomena at the Landau levels (embedded in the spectrum) are more complicated to analyse. It can be done in several ways.

In the case of potential perturbations such phenomena are justified by proving that the Landau levels are singularities of the Spectral Shift Function (see [11]) on one hand and on the other hand that the Landau levels are accumulation points of resonances (see [4], [5]). It is also possible to prove that some axisymmetric perturbations can produce an infinite number of embedded eigenvalues near the Landau levels (see [6]). Let us mention that, below the first Landau level, where the resonances are only eigenvalues and, up to a sign, the Spectral Shift Function is the counting function of eigenvalues, these results coincide.

In view of the results in the 2D case, a natural conjecture for the 3D exterior problems, is that the clusters phenomena for the Dirichlet (resp. Robin or Neumann) operator are close to those established for $H_0 + \mathbb{1}_K$ (resp. $H_0 - \mathbb{1}_K$). Before discussing the obstacle problems, let us recall the known results for $H_\pm := H_0 \pm \mathbb{1}_K$, with $\mathbb{1}_K$ the multiplication operator by the characteristic function of the compact set K having a non-empty interior.

3.2. Singularities of the Spectral Shift Function for perturbations by characteristic functions

We consider K having a non-empty interior and $\mathbb{1}_K$ being the multiplication operator by the characteristic function of K. Introduce the self-adjoint operator

$$H_\pm := H_0 \pm \mathbb{1}_K.$$

It is well known that since the resolvent difference $(H_\pm - i)^{-1} - (H_0 - i)^{-1}$ is a trace-class operator, there exists a unique

$$\xi = \xi(\cdot; H_\pm, H_0) \in L^1(\mathbb{R}; (1 + E^2)^{-1} dE)$$

such that the Lifshits–Krein trace formula

$$\mathrm{Tr}\,(f(H_\pm) - f(H_0)) = \int_{\mathbb{R}} \xi(E; H_\pm, H_0) f'(E) dE$$

holds for each $f \in C_0^\infty(\mathbb{R})$ and the normalization condition $\xi(E; H_\pm, H_0) = 0$ is fulfilled for each $E \in (-\infty, \inf \sigma(H_\pm))$ (see the original works [18, 17] or [24, Chapter 8]).

The function $\xi(\cdot; H_\pm, H_0)$ is called *the spectral shift function* (SSF) for the operator pair $(H_\pm, H_0)$. By the *Birman–Krein formula*, for almost every $E > b$, it coincides with *the scattering phase* for the operator pair $(H_\pm, H_0)$ (see the original work [3] or the monograph [24]).
Further, for almost every $E < b$ we have

$$-\xi(E; H_\pm, H_0) = \#\{eig.(H_\pm) \in (-\infty, E)\}.$$

By [7, Proposition 2.5], the SSF for the operator pair $(H_\pm, H_0)$ is bounded on every compact subset of $\mathbb{R} \setminus \{\Lambda_q;\ q \geq 0\}$ and is continuous on $\mathbb{R} \setminus (\{\Lambda_q;\ q \geq 0\} \cup \sigma_{\mathrm{pp}}(H_\pm))$ where $\sigma_{\mathrm{pp}}(H_\pm)$ is the set of the eigenvalues of $H_\pm$. Moreover, since the characteristic function $\mathbb{1}_K$ is compactly supported, the analysis of the SSF in terms of resonances (see Section 5 of [4]) proves the analyticity of $\xi(\cdot; H_\pm, H_0)$ on $\mathbb{R} \setminus (\{\Lambda_q;\ q \geq 0\} \cup \sigma_{\mathrm{pp}}(H_\pm))$.

In [11], Fernandez–Raikov describe the asymptotic behavior of the SSF $\xi(E; H_\pm, H_0)$ as $E \to \Lambda_q$ for potentials admitting a power-like decay, an exponential decay, or having a compact support. In particular for the pair $(H_\pm, H_0)$ they obtain:

Theorem 3.1 ([11, Theorems 3.1, 3.2]). *Fix $q \in \mathbb{N}$. Then as $\lambda \downarrow 0$, we have*

$$\begin{aligned} \xi(\Lambda_q - \lambda; H_+, H_0) &= O(1), \\ \xi(\Lambda_q + \lambda; H_+, H_0) &\sim \quad |\ln r| \, (4 \ln |\ln r|)^{-1}, \\ \xi(\Lambda_q - \lambda; H_-, H_0) &\sim -|\ln r| \, (2 \ln |\ln r|)^{-1}, \\ \xi(\Lambda_q + \lambda; H_-, H_0) &\sim -|\ln r| \, (4 \ln |\ln r|)^{-1}. \end{aligned}$$

These above results suggest the following conjecture for the exterior problem, but, to our best knowledge, it is still not proved:

Conjecture. Fix $q \in \mathbb{N}$. As $\lambda \downarrow 0$,

$$\begin{aligned} \xi(\Lambda_q - \lambda; H_\Omega^\infty, H_0) &= O(1), \\ \xi(\Lambda_q + \lambda; H_\Omega^\infty, H_0) &\sim \quad |\ln r| \, (4 \ln |\ln r|)^{-1}, \\ \xi(\Lambda_q - \lambda; H_\Omega^\gamma, H_0) &\sim -|\ln r| \, (2 \ln |\ln r|)^{-1}, \\ \xi(\Lambda_q + \lambda; H_\Omega^\gamma, H_0) &\sim -|\ln r| \, (4 \ln |\ln r|)^{-1}. \end{aligned}$$

3.3. Clusters of resonances

In order to define the resonances, let us recall analytic properties of the free resolvent. Let $\mathcal{M}$ be the connected infinite-sheeted covering of $\mathbb{C} \setminus \cup_{q\in\mathbb{N}}\{\Lambda_q\}$ where each function $z \mapsto \sqrt{z - \Lambda_q}$, $q \in \mathbb{N}$, is analytic. Near a Landau level Λ_q, this Riemann surface $\mathcal{M}$ can be parametrized by $z_q(k) = \Lambda_q + k^2$, $k \in \mathbb{C}^*$, $|k| \ll 1$ (for more details, see Section 2 of [4]). For $\epsilon > 0$, we denote by $\mathcal{M}_\epsilon$ the set of the points $z \in \mathcal{M}$ such that for each $q \in \mathbb{N}$, we have $\operatorname{Im}\sqrt{z - \Lambda_q} > -\epsilon$. We have $\cup_{\epsilon>0}\mathcal{M}_\epsilon = \mathcal{M}$.

Proposition 3.2 ([4, Proposition 1]). *For each $\epsilon > 0$, the operator-valued function $z \mapsto R_0(z)$,*

$$R_0(z) = (H_0 - z)^{-1} : e^{-\epsilon\langle x_3\rangle} L^2(\mathbb{R}^3) \to e^{\epsilon\langle x_3\rangle} L^2(\mathbb{R}^3)$$

has a holomorphic extension (still denoted by $R_0(z)$) from the open upper half-plane $\mathbb{C}_+ := \{z \in \mathbb{C};\ \operatorname{Im} z > 0\}$ to $\mathcal{M}_\epsilon$.

Let p_q be the orthogonal projection onto $\ker(H_{\text{Landau}} - \Lambda_q)$. Thanks to the orthogonal decomposition of $(H_0 - z)^{-1}$:

$$(H_0 - z)^{-1} = \sum_{q\in\mathbb{N}} p_q \otimes (D_{x_3}^2 + \Lambda_q - z)^{-1},$$

the above result is a consequence of the holomorphic extension of $z \mapsto (D_{x_3}^2 + \Lambda_q - z)^{-1}$ whose integral kernel is $\frac{e^{-\sqrt{\Lambda_q - z}|x_3 - x_3'|}}{2\sqrt{\Lambda_q - z}}$.

Then, by using some resolvent equations and the analytic Fredholm theorem, from Proposition 3.2, we deduce meromorphic extension of the resolvents of H_Ω^∞ and H_Ω^γ (see Section 3 of [8]).

We are able to define the resonances:

Definition 3.3. For $\bullet = \infty, \gamma$, we define the resonances for $H_\Omega^\bullet$ as the poles of the meromorphic extension of the resolvent

$$R_\Omega^\bullet(z) := (H_\Omega^\bullet - z)^{-1} : e^{-\epsilon\langle x_3\rangle} L^2(\Omega) \to e^{\epsilon\langle x_3\rangle} L^2(\Omega).$$

These poles (i.e., the resonances) and the rank of their residues (the multiplicity of the resonance) do not depend on $\epsilon > 0$.

Note that in dimension 2 the analog of Proposition 3.2 is trivial (for $\epsilon \geq 0$), because the free Hamiltonian H_{Landau} has no spectrum outside the Landau levels. In this case, the poles of the Definition 3.3, for $\epsilon = 0$ are simply the eigenvalues of the 2D exterior problems.

The study of the distribution of the resonances of H_Ω^∞ and H_Ω^γ near the Landau levels is done in our recent work [8]. We obtained that the distribution of the resonances of H_Ω^∞ (resp. H_Ω^γ) near the Landau levels is essentially governed by the distribution of resonances of $H_0 + \mathbb{1}_K$ (resp. $H_0 - \mathbb{1}_K$) which is known thanks to [5].

More precisely, as stated in the following results, we have a localization of the resonances of H_Ω^∞ and H_Ω^γ near the Landau levels Λ_q, $q \in \mathbb{N}$, together with an asymptotic expansion of the resonances counting function in the small annulus adjoining Λ_q, $q \in \mathbb{N}$. As consequences we obtain some information concerning eigenvalues.

For an operator H and $q \in \mathbb{N}$ fixed, let us introduce the counting function of resonances near Λ_q:

$$\mathcal{N}_q(H, r, r_0) := \#\{z_q(k) = \Lambda_q + k^2 \in res.(H);\ \sqrt{r} < |k| < \sqrt{r_0}\},\quad 0 < r < r_0 < 2b. \tag{3.2}$$

Theorem 3.4. *Let $K \subset \mathbb{R}^3$ be a smooth compact domain. Fix a Landau level Λ_q, $q \in \mathbb{N}$, such that K does not produce an isolated resonance at Λ_q.*

Then the resonances $z_q(k) = \Lambda_q + k^2$ of H_Ω^∞ and H_Ω^γ, with $|k| \ll 1$ sufficiently small, satisfy:

(i) *For the Dirichlet exterior problem ($\bullet = \infty$), the resonances z_q are far from the z-real axis in the sense that there exists $r_0 > 0$ such that $k = \sqrt{z_q - \Lambda_q}$, $|k| < r_0$ satisfies:*

$$\text{Im}(k) \leq 0, \qquad \text{Re}(k) = o(|k|).$$

(ii) *For the Neumann–Robin exterior problem ($\bullet = \gamma$), the resonances z_q are close to the real axis, below Λ_q, in the sense that there exists $r_0 > 0$ such that $k = \sqrt{z_q - \Lambda_q}$, $|k| < r_0$ satisfies:*

$$\text{Im}(k) \geq 0, \qquad \text{Re}(k) = o(|k|).$$

And for $\bullet = \infty, \gamma$ *and* r_0 *fixed, the following asymptotics holds for counting function of resonances*

$$\mathcal{N}_q(H_\Omega^\bullet, r, r_0) \sim \frac{|\ln r|}{2\ln|\ln r|}\big(1 + o(1)\big), \qquad r \searrow 0.$$

In particular, near the first Landau level $\Lambda_0 = b$, using that the only poles $z_0(k) = \Lambda_0 + k^2$, with $\mathrm{Im} k > 0$, are the eigenvalues below Λ_0 (for which $\mathrm{Re}(k) = 0$), and the fact that the Dirichlet operator is a non-negative perturbation of H_0 (see Lemma 4.3), we have:

Corollary 3.5.

(i) *The Robin (resp. Neumann) exterior operator* H_Ω^γ *(resp.* H_Ω^0*) has an increasing sequence of eigenvalues* $\{\mu_j\}_j$ *which accumulate at* Λ_0 *with the distribution:*

$$\#\{\mu_j \in \sigma_p(H_\Omega^\gamma) \cap (-\infty, \Lambda_0 - \lambda)\} \sim \frac{|\ln \lambda|}{2\ln|\ln \lambda|}\big(1 + o(1)\big), \qquad \lambda \searrow 0.$$

(ii) *The Dirichlet exterior operator* H_Ω^∞ *has no eigenvalues below* Λ_0*.*

Remark. Since, on the point spectrum, the Spectral Shift Function coincides with the counting function of the eigenvalues (up to a sign), then Corollary 3.5 shows that the above conjecture is true at the energies below Λ_0.

Moreover, since the embedded eigenvalues of the operator $H_\Omega^\bullet$ in $[b, +\infty) \setminus \cup_{q=0}^\infty \{\Lambda_q\}$ are the resonances $z_q(k)$ with $k \in e^{i\{0,\frac{\pi}{2}\}}(0, \sqrt{2b})$, then, for each $q \in \mathbb{N}$, an immediate consequence of Theorem 3.4 (i) and (ii) is the absence of embedded eigenvalues of H_Ω^∞ in $(\Lambda_q - r_0^2, \Lambda_q) \cup (\Lambda_q, \Lambda_q + r_0^2)$ and of embedded eigenvalues of H_Ω^γ in $(\Lambda_q, \Lambda_q + r_0^2)$, for r_0 sufficiently small. Hence we have the following result:

Corollary 3.6. *In* $[b, +\infty) \setminus \cup_{q=0}^\infty \{\Lambda_q\}$ *(resp. in* $[b, +\infty) \setminus \cup_{q=1}^\infty \{(\Lambda_q - r_0^2, \Lambda_q)\}$*),* $r_0 > 0$*, the embedded eigenvalues of the operator* H_Ω^∞ *(resp.* H_Ω^γ*), form a discrete set.*

Let us recall that the above results concerning the distribution of resonances of H_Ω^∞ (resp. H_Ω^γ) are exactly the same for the resonances of $H_0 + \mathbb{1}_K$ (resp. $H_0 - \mathbb{1}_K$) (see [22] for the eigenvalues below Λ_0, and [4], [5] for resonances near the Landau levels).

In comparison with previous works, the spectral study of obstacle perturbations in the 3D case leads to two new difficulties. The first, with respect to the 2D case, comes from the presence of continuous spectrum, then the spectral study involves resonances and some non-selfadjoint aspects. The second difficulty, with respect to the potential perturbations, is due to the fact that the perturbed and the unperturbed operators are not defined on the same space.

4. Idea of the proof

In this section we give the main steps of the proofs of the results of Section 3. For detailed proofs, we refer to [8]. As written above, an important difficulty, with

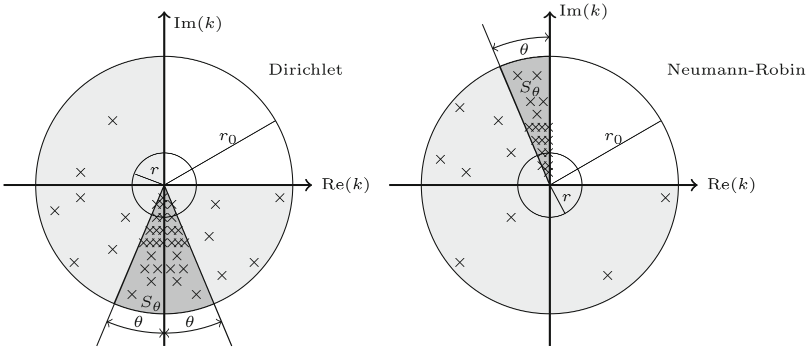

FIGURE 1. **Localization of the resonances in variable** k**:** For r_0 sufficiently small, the resonances $z_q(k) = \Lambda_q + k^2$ of the operators $H_\Omega^\bullet$, $\bullet = \infty, \gamma$, near a Landau level Λ_q, $q \in \mathbb{N}$, are concentrated in the sectors S_θ. For $\bullet = \infty$ they are concentrated near the semi-axis $-i(0, +\infty)$ in both sides, while they are concentrated near the semi-axis $i(0, +\infty)$ on the left for $\bullet = \gamma$.

respect to the potential perturbations, is due to the fact that the perturbed and the unperturbed operators are not defined on the same space. In order to overcome this difficulty, first we introduce an appropriate perturbation $V^\bullet$, $\bullet = \infty, \gamma$, of H_0^{-1} on $L^2(\mathbb{R}^3)$.

4.1. Auxiliary operators and characterization of the resonances

By identification of $L^2(\mathbb{R}^3)$ with $L^2(\Omega) \oplus L^2(K)$, we consider the following operators in $L^2(\mathbb{R}^3)$:

$$\tilde{H}^\gamma := H_\Omega^\gamma \oplus H_K^{-\gamma} \qquad \text{on} \qquad \mathrm{Dom}(H_\Omega^\gamma) \oplus \mathrm{Dom}(H_K^{-\gamma}), \tag{4.1}$$

where $H_K^{-\gamma}$ is the Robin operator in K. Namely, $H_K^{-\gamma}$ is the self-adjoint operator associated with the closure of the quadratic form $Q_K^{-\gamma}$ defined by (1.2), by replacing γ and Ω with $-\gamma$ and K respectively. The spectrum of this elliptic operator $H_K^{-\gamma}$, on $L^2(K)$ with K compact, is discrete and its eigenvalues, arranged in increasing order, tend to infinity.

Without loss of generality, we can assume that H_Ω^γ, $H_K^{-\gamma}$ and H_Ω^∞ are positive and invertible (if not, it is sufficient to shift them by the same constant), and we introduce

$$V^\gamma := H_0^{-1} - (\tilde{H}^\gamma)^{-1} = H_0^{-1} - (H_\Omega^\gamma)^{-1} \oplus (H_K^{-\gamma})^{-1}, \tag{4.2}$$

$$V^\infty := H_0^{-1} - (H_\Omega^\infty)^{-1} \oplus 0. \tag{4.3}$$

Let us introduce, for $\mathrm{Im}(z) > 0$, the resolvent operators

$$\tilde{R}^\gamma(z) = (\tilde{H}^\gamma - z)^{-1} = (H_\Omega^\gamma - z)^{-1} \oplus (H_K^{-\gamma} - z)^{-1} \quad \text{and} \quad \tilde{R}^\infty(z) = (H_\Omega^\infty - z)^{-1} \oplus 0. \tag{4.4}$$

From the above properties, it is clear that for $\bullet = \gamma, \infty$, the operator-valued function

$$\tilde{R}^\bullet(z) : e^{-\epsilon\langle x_3\rangle} L^2(\mathbb{R}^3) \longrightarrow e^{\epsilon\langle x_3\rangle} L^2(\mathbb{R}^3)$$

has a meromorphic extension $\big($also denoted $\tilde{R}^\bullet(\cdot)\big)$ from the open upper half-plane to $\mathcal{M}_\epsilon$, $\epsilon < \sqrt{b}$ and according to their multiplicities (i.e., the rank of their residues), the poles of R^∞_Ω coincide with the poles of $\tilde{R}^\infty$ and the poles of R^γ_Ω are those of $\tilde{R}^\gamma$ excepted the eigenvalues of $H_K^{-\gamma}$. In particular, since the spectrum of $H_K^{-\gamma}$ is discrete, we have:

Proposition 4.1. *For* $0 < r_0 < 2b$ *fixed, the counting function of resonances* (*see Definition* (3.2)) *satisfies:*

$$\mathcal{N}_q(H^\infty_\Omega, r, r_0) = \#\{z_q(k) = \Lambda_q + k^2 \textit{ pole of } \tilde{R}^\infty;\ \sqrt{r} < |k| < \sqrt{r_0}\},$$
$$\mathcal{N}_q(H^\gamma_\Omega, r, r_0) = \#\{z_q(k) = \Lambda_q + k^2 \textit{ pole of } \tilde{R}^\gamma;\ \sqrt{r} < |k| < \sqrt{r_0}\} \ + \ O(1)$$

uniformly with respect to $r \in (0, r_0)$.

Then, for $\bullet = \infty, \gamma$, the clusters phenomena for the resonances of $H^\bullet_\Omega$ near Λ_q are reduced to the accumulation properties of the poles of $\tilde{R}^\bullet$ at Λ_q. Moreover from some Birman–Schwinger type arguments, we obtain that z is a pole of $\tilde{R}^\bullet$ if and only if (-1) is an eigenvalue of the analytic extension of

$$\begin{aligned} B^\bullet(z) &:= \operatorname{sign}(V^\bullet)\,|V^\bullet|^{\frac12} \left(\frac{1}{z} - H_0^{-1}\right)^{-1} |V^\bullet|^{\frac12} \\ &= \operatorname{sign}(V^\bullet)\,|V^\bullet|^{\frac12}\, zH_0(H_0 - z)^{-1}|V^\bullet|^{\frac12} \\ &= zV^\bullet + z^2\operatorname{sign}(V^\bullet)\,|V^\bullet|^{\frac12}\,(H_0 - z)^{-1}|V^\bullet|^{\frac12} \end{aligned}$$

and we have:

Proposition 4.2 ([8], Proposition 3.3). *For* $\bullet = \infty, \gamma$, *the following assertions are equivalent:*

a) z *is a pole of* $\tilde{R}^\bullet$ *in* $\mathcal{L}\Big(e^{-\epsilon\langle x_3\rangle} L^2(\mathbb{R}^3), e^{\epsilon\langle x_3\rangle} L^2(\mathbb{R}^3)\Big)$,

b) z *is a pole of* $|V^\bullet|^{\frac12}\tilde{R}^\bullet|V^\bullet|^{\frac12}$ *in* $\mathcal{L}\Big(L^2(\mathbb{R}^3)\Big)$,

c) -1 *is an eigenvalue of* $B^\bullet(z)$ *with*

$$B^\bullet(z) := zV^\bullet + z^2\operatorname{sign}(V^\bullet)\,|V^\bullet|^{\frac12}\,(H_0 - z)^{-1}|V^\bullet|^{\frac12}. \tag{4.5}$$

The above results allow us to reduce our problem to the analysis of the complex numbers $z_q \in \mathcal{M}$ such that $I + B^\bullet_q(z_q)$ is not invertible. The study of these so-called *characteristic values* of the holomorphic operator-valued function $I + B^\bullet_q$ will be done exploiting tools of [5] (see Proposition 4.5 below). In particular, we use that the perturbation $V^\bullet$ is of definite sign and some properties of the restriction of $V^\bullet$ to the space of functions f satisfying $(H_0 - \Lambda_q)f = 0$ near K.

4.2. Properties of $V^\bullet$

From the analysis of the quadratic forms (and of their domains) associated with V^∞ and V^γ we easily obtain:

Lemma 4.3 ([8], Lemma 3.1). *The operators V^∞ and V^γ defined by* (4.3) *and* (4.2) *are respectively non-negative and non-positive compact operators in $\mathcal{L}(L^2(\mathbb{R}^3))$.*

Let us introduce a compact domain $K_1 \subset \mathbb{R}^3$ which contains K and

$$\mathcal{E}_q(K_1) = \big\{ f \in L^2(\mathbb{R}^3) \cap C^\infty(\mathbb{R}^3);\ (H_0 - \Lambda_q) f = 0 \text{ on } K_1 \big\}. \tag{4.6}$$

Proposition 4.4 ([8], Proposition 5.1). *Fix K_0, K_1 two compact domains of $\mathbb{R}^3$, $K_0 \subset K \subset K_1$ with $\partial K_i \cap \partial K = \emptyset$, $i = 0, 1$. For $\bullet = \infty, \gamma$, there exists $\mathcal{L}_q$, a finite codimension subspaces of $\mathcal{E}_q(K_1)$ and $C > 1$ such that for any $f \in \mathcal{L}_q$,*

$$\frac{1}{C} \langle f, \mathbb{1}_{K_0} f \rangle_{L^2(\mathbb{R}^3)} \leq \langle H_0 f,\, |V^\bullet|\, H_0 f \rangle_{L^2(\mathbb{R}^3)} \leq C \langle f, \mathbb{1}_{K_1} f \rangle_{L^2(\mathbb{R}^3)}, \qquad \bullet = \infty, \gamma. \tag{4.7}$$

The proof of this result is the object of Sections 5 and 6 of [8]. The lower bound in the Dirichlet case is inspired by the analogous result in the 2D case (see Proposition 3.1 of [21]). It exploits the resolvent equation

$$H_0^{-1} - (H_0 + \mathbb{1}_{K_0})^{-1} = H_0^{-1} \mathbb{1}_{K_0} \Big(I - \mathbb{1}_{K_0} (H_0 + \mathbb{1}_{K_0})^{-1} \mathbb{1}_{K_0} \Big) \mathbb{1}_{K_0} H_0^{-1},$$

and the fact that $\mathbb{1}_{K_0}(H_0 + \mathbb{1}_{K_0})^{-1}\mathbb{1}_{K_0}$ is a compact operator in $\mathcal{L}(L^2(\mathbb{R}^3))$. The proof of the other estimates (lower bound for $\bullet = \gamma$ and upper bounds) is closely related to the 2D case (see Lemma 4.2 of [13]). It exploits the expressions of $V^\bullet$ in terms of *Dirichlet–Neumann* and *Robin–Dirichlet* operators and their elliptic properties as pseudo-differential operators on Σ.

For T a compact self-adjoint operator, let us introduce the counting function

$$n(r, T) := \operatorname{Tr} \mathbb{1}_{[r, +\infty)}(T), \tag{4.8}$$

the number of eigenvalues of the operator T lying in the interval $[r, +\infty) \subset \mathbb{R}^*$, counted with their multiplicity. In the following, we will use the asymptotic properties of the counting function for the Toeplitz operator $p_q W^\bullet p_q$, where $W^\bullet$ is the operator defined on $L^2(\mathbb{R}^2)$ by:

$$(W^\bullet f^\perp)(x_1, x_2) = \frac{1}{2} \int_{\mathbb{R}_{x_3}} \Big(|V^\bullet| (f^\perp \otimes 1_{\mathbb{R}}) \Big)(x_1, x_2, x_3) dx_3. \tag{4.9}$$

From the min-max principle and Proposition 4.4, we deduce there exists $C > 1$, such that:

$$n\big(Cr, p_q \mathbb{1}_{K_0^\perp} p_q\big) \leq n\big(r, p_q W^\bullet p_q\big) \leq n\big(r/C, p_q \mathbb{1}_{K_1^\perp} p_q\big), \tag{4.10}$$

where $K_0^\perp$ and $K_1^\perp$ are compact sets (with nonempty interior) such that $K_0^\perp \times I_0 \subset K \subset K_1^\perp \times I_1$ for some intervals I_0, I_1.

According to [23, Lemma 3.5], for $i = 0, 1$, we have

$$n\big(r, p_q \mathbb{1}_{K_i^\perp} p_q\big) = \frac{|\ln r|}{\ln|\ln r|}\big(1 + o(1)\big) \quad \text{as} \quad r \searrow 0.$$

Then, we deduce

$$n\big(r, p_q W^\bullet p_q\big) = \frac{|\ln r|}{\ln|\ln r|}\big(1 + o(1)\big), \qquad r \searrow 0. \tag{4.11}$$

4.3. Proof of Theorem 3.4

From Proposition 4.1 and Proposition 4.2, for $\bullet = \infty, \gamma$, we have:

$$\begin{aligned}\mathcal{N}_q(H_\Omega^\bullet, r, r_0) = \#\big\{ z_q(k) = \Lambda_q + k^2,\ \sqrt{r} < |k| < \sqrt{r_0},\ \text{such that} \\ I + B^\bullet(z_q(k)) \text{ is not invertible}\big\} \ +\ O(1)\end{aligned}$$

uniformly with respect to $r \in (0, r_0]$.

The operator $V^\bullet$ is of fixed sign (see Lemma 4.3) and exploiting (4.11), $k = 0$ is a pole of $k \mapsto B^\bullet(z_q(k))$ with the residue $A_q^\bullet(0) := \lim_{k\to 0} ikB^\bullet(z_q(k))$ satisfying:

$$n\big(r, |A_q^\bullet(0)|\big) = n\big(r, \Lambda_q^2 p_q W^\bullet p_q\big) = \frac{|\ln r|}{\ln|\ln r|}\big(1 + o(1)\big), \qquad r \searrow 0 \tag{4.12}$$

(see Proposition 4.3 of [8] or previous results [4, 5]). Then, we conclude the proof of Theorem 3.4 from Proposition 4.5 below (applied with $z = ik$), provided the invertibility of $I - A'(0)\Pi_0$ holds. For a more complete interpretation and discussion on this latter assumption we refer to Section 4.4 of [8]. In the statement of Theorem 3.4, it is expressed by K *does not produce an isolated resonance* (*or eigenvalue*) *at* Λ_q. We can hope that this hypothesis is generic, for instance in the sense that, if it does not hold for some K, then, under a small perturbation of the obstacle K, it becomes true.

Proposition 4.5 ([5], [8] Proposition 4.2). *For $\mathcal{D}$ a domain of $\mathbb{C}$ containing zero, and S_∞ the class of compact operators in a separable Hilbert space, we consider a holomorphic operator-valued function $A : \mathcal{D} \longrightarrow S_\infty$ and introduce the set of the characteristic values of $\big(I - \frac{A(z)}{z}\big)$ inside $\Delta \Subset \mathbb{C} \setminus \{0\}$:*

$$\mathcal{Z}(\Delta, A) := \left\{ z \in \Delta : I - \frac{A(z)}{z} \text{ is not invertible} \right\}.$$

Assume that $A(0)$ is self-adjoint and $\mathcal{Z}(\Delta, A)$ is non-empty. Denote by Π_0 the orthogonal projection onto $\ker A(0)$ and assume that $I - A'(0)\Pi_0$ is invertible.

If $\Delta \Subset \mathbb{C} \setminus \{0\}$ is a bounded domain with smooth boundary $\partial\Delta$ which is transverse to the real axis at each point of $\partial\Delta \cap \mathbb{R}$, then we have:

(i) *The characteristic values $z \in \mathcal{Z}(\Delta, A)$ near 0 satisfy $|\mathrm{Im}(z)| = o(|z|)$ as $|z|$ tends to 0.*

(ii) *If the operator $A(0)$ has a definite sign ($\pm A(0) \geq 0$), then the characteristic values z near 0 satisfy $\pm\mathrm{Re}(z) \geq 0$.*

(iii) *For* $\pm A(0) \geq 0$*, if the counting function of* $A(0)$*,*

$$n(r, \pm A(0)) := \operatorname{Tr} \mathbb{1}_{[r,+\infty)}(\pm A(0))$$

satisfies:

$$n(r, \pm A(0)) = c_0 \frac{|\ln r|}{\ln|\ln r|}(1 + o(1)), \qquad r \searrow 0,$$

then, for $r_0 > 0$ *fixed, the counting function of the characteristic values near* 0 *satisfies:*

$$\#\big\{z \in \mathcal{Z}(\Delta, A);\ r < |z| < r_0\big\} = c_0 \frac{|\ln r|}{\ln|\ln r|}(1 + o(1)), \qquad r \searrow 0,$$

where the multiplicity of a characteristic value z_0 *is defined by*

$$\operatorname{mult}(z_0) := \frac{1}{2i\pi} \operatorname{tr}\left(\int_{\mathcal{C}} \left(-\frac{A(z)}{z}\right)' \left(I - \frac{A(z)}{z}\right)^{-1} dz \right).$$

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The Spectral Shift Function and the Witten Index

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Abstract. We survey the notion of the spectral shift function of two operators and recent progress on its connection with the Witten index. We begin with classical definitions of the spectral shift function $\xi(\,\cdot\,; H_2, H_1)$ under various assumptions on the pair of operators (H_2, H_1) in a fixed Hilbert space and then discuss some of its properties. We then present a new approach to defining the spectral shift function and discuss Krein's Trace Theorem. In particular, we describe a proof that does not use complex analysis [53] and develop its extension to general σ-finite von Neumann algebras $\mathcal{M}$ of type II and unbounded perturbations from the predual of $\mathcal{M}$.

We also discuss the connection between the theory of the spectral shift function and index theory for certain model operators. We start by introducing various definitions of the Witten index, (an extension of the notion of Fredholm index to non-Fredholm operators). Then we study the model operator $\boldsymbol{D}_{\boldsymbol{A}} = (d/dt) + \boldsymbol{A}$ in $L^2(\mathbb{R}; \mathcal{H})$ associated with the operator path $\{A(t)\}_{t=-\infty}^{\infty}$, where $(\boldsymbol{A}f)(t) = A(t)f(t)$ for a.e. $t \in \mathbb{R}$, and appropriate $f \in L^2(\mathbb{R}; \mathcal{H})$ (with $\mathcal{H}$ being a separable, complex Hilbert space). The setup permits the operator family $A(t)$ on $\mathcal{H}$ to be an unbounded relatively trace class perturbation of the unbounded self-adjoint operator A_-, and no discrete spectrum assumptions are made on the asymptotes $A_\pm$.

When there is a spectral gap for the operators $A_\pm$ at zero, it is shown that the operator $\boldsymbol{D}_{\boldsymbol{A}}$ is Fredholm and the Fredholm index can be computed as

$$\operatorname{ind}(\boldsymbol{D}_{\boldsymbol{A}}) = \xi(0_+; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2) = \xi(0; A_+, A_-).$$

When $0 \in \sigma(A_+)$ (or $0 \in \sigma(A_-)$), the operator $\boldsymbol{D}_{\boldsymbol{A}}$ ceases to be Fredholm. However, under the additional assumption that 0 is a right and a left Lebesgue point of $\xi(\,\cdot\,; A_+, A_-)$, it is proved that 0 is also a right Lebesgue point of $\xi(\,\cdot\,; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2)$. For the resolvent (resp., semigroup) regularized Witten index $W_r(\boldsymbol{D}_{\boldsymbol{A}})$ (resp., $W_s(\boldsymbol{D}_{\boldsymbol{A}})$) the following equality holds,

$$\begin{aligned} W_r(\boldsymbol{D}_{\boldsymbol{A}}) = W_s(\boldsymbol{D}_{\boldsymbol{A}}) &= \xi(0_+; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2) \\ &= [\xi(0_+; A_+, A_-) + \xi(0_-; A_+, A_-)]/2. \end{aligned}$$

We also study a special example, when the perturbation of the unbounded self-adjoint operator A_- is not assumed to be relatively trace class.

In this example $A_- = -i\frac{d}{dx}$ is the differentiation operator on $L^2(\mathbb{R})$ and the perturbation is given by the multiplication operator by a (bounded) real-valued function f on $\mathbb{R}$. Under certain assumptions on f it is proved that

$$\begin{aligned} W_r(\boldsymbol{D_A}) = W_s(\boldsymbol{D_A}) &= \xi(0_+; \boldsymbol{D_A}\boldsymbol{D_A^*}, \boldsymbol{D_A^*}\boldsymbol{D_A}) \\ &= \xi(0; A_+, A_-) = \frac{1}{2\pi}\int_{\mathbb{R}} f(s)\,ds. \end{aligned}$$

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Contents

1. Introduction

The purpose of this article is twofold: We give a detailed survey of the Lifshitz–Krein spectral shift function and its properties, and we then review the notion of the Witten index and its relation to the spectral shift function and to spectral flow.

We begin in Section 2 with an account of the history of the spectral shift function starting with the work of Lifshitz and Krein. We discuss several points of view on the definition and then move on to more recent developments. We explain in some detail a recent real analysis approach to the fundamental theorem of Krein (almost all complete earlier proofs use complex analysis, see, however, [57] and [60]). The novelty here is that the proof also applies when one works in the generality of semifinite von Neumann algebras (rather than just the algebra of bounded operators on a Hilbert space).

Starting in Section 3 we survey the properties of the Witten index from a more contemporary perspective. We introduce a special "supersymmetric" model operator motivated by geometric considerations. We describe in Section 4 recent results relevant to index theory that do not depend on assuming that the operators under study all have discrete spectrum. In particular, we focus on two formulae (we call these the principle trace formula and the Pushnitski formula) that seem especially interesting. Generalizations of both of these formulae are described in terms of recent results (published and, as of yet, unpublished ones). We briefly explain in the final section some new examples that point the way to higher-dimensional examples.

2. Spectral shift function

In 1947, the well-known physicist I.M. Lifshitz considered perturbations of an operator H_0 (arising as the Hamiltonian of a lattice model in quantum mechanics) by a finite-rank perturbation V and found some formulae and quantitative relations for the size of the shift of the eigenvalues. In one of his papers the spectral shift function (SSF), $\xi(\,\cdot\,; H_0+V, H_0)$, appeared for the first time, and formulae for it in the case of a finite-rank perturbation were obtained.

Lifshitz later continued these investigations and applied them to the problem of computing the trace of the operator $\phi(H_0+V)-\phi(H_0)$, where H_0 is the unperturbed self-adjoint operator, V is a self-adjoint, finite-dimensional perturbation, acting on the same Hilbert space $\mathcal{H}$, and ϕ is an appropriate function (belonging to a fairly broad class). He obtained (or, rather, surmised) the remarkable relation

$$\operatorname{tr}_{\mathcal{H}}(\phi(H_0+V)-\phi(H_0)) = \int_{\mathbb{R}} \phi'(\lambda)\xi(\lambda; H_0+V, H_0)\, d\lambda, \tag{2.1}$$

where the function $\xi(\,\cdot\,; H_0+V, H_0)$ depends on operators H_0 and V only.

A physical example treated by Lifshitz is the following: if H_0 is the operator describing the oscillations of a crystal lattice, then the free energy of the oscillations can be represented in the form $F = \operatorname{tr}_{\mathcal{H}}(\phi(H_0))$, for some ϕ. In this case, the trace formula enables one to compute the change in the free energy of oscillations of the crystal lattice upon introduction of a foreign admixture into the crystal.

If one wants to study continuous analogues of lattice models, perturbations V, as a rule, are no longer described by finite-rank operators. For such models the appropriate class of perturbations, such that the spectral shift function may be defined, needs to be described. In his paper [43], M.G. Krein resolved this problem. Furthermore, he described the broad class of functions ϕ for which (2.1) holds. His approach was based on the notion of perturbation determinants to be discussed next.

2.1. Perturbation determinants

Let $\mathcal{H}$ be a complex, separable Hilbert space, $\mathcal{B}(\mathcal{H})$ be the algebra of all bounded linear operators in $\mathcal{H}$ equipped with the uniform norm $\|\cdot\|_\infty$ and let $\mathcal{B}_1(\mathcal{H})$ be the ideal of all trace class operators, equipped with the the norm $\|\cdot\|_1$. The latter ideal, besides carrying the standard trace $\operatorname{tr}_{\mathcal{H}}(\cdot)$, also gives rise to the notion of a determinant, which generalizes the corresponding notion in the finite-dimensional case. Let $T \in \mathcal{B}_1(\mathcal{H})$. For any orthonormal basis $\{\omega_n\}_{n\in\mathbb{N}}$ in $\mathcal{H}$ consider the $N \times N$ matrix $\mathcal{T}_N$ with elements $\delta_{m,n} + (T\omega_m, \omega_n)$, $m, n \in 1, \dots, N$. Then the following limit exists:

$$\lim_{N\to\infty} \det(I + \mathcal{T}_N) =: \det_{\mathcal{H}}(I + T)$$

independently of the choice of the basis $\{\omega_n\}_{n\in\mathbb{N}}$ (cf., [33, Ch. IV]). The functional $\det_{\mathcal{H}}(I + \cdot\,) : \mathcal{B}_1(\mathcal{H}) \to \mathbb{C}$ is called the *determinant*; it is continuous with respect to the $\mathcal{B}_1(\mathcal{H})$-norm.

In terms of eigenvalues of $T \in \mathcal{B}_1(\mathcal{H})$, $\{\lambda_k(T)\}_{k\in\mathcal{I}}$, $\mathcal{I} \subseteq \mathbb{N}$, an appropriate index set, one has

$$\det_{\mathcal{H}}(I + T) = \prod\nolimits_{k\in\mathcal{I}} (1 + \lambda_k(T)),$$

where the product converges absolutely (due to the fact that $\sum_{k\in\mathcal{I}} |\lambda_k| < \infty$). We note the following properties of the determinant [33]:

$$\begin{aligned}
\det_{\mathcal{H}}(I + T^*) &= \overline{\det_{\mathcal{H}}(I + T)}, && T \in \mathcal{B}_1(\mathcal{H}),\\
\det_{\mathcal{H}}\big((I + T_1)(I + T_2)\big) &= \det_{\mathcal{H}}(I + T_1)\det_{\mathcal{H}}(I + T_2), && T_1, T_2 \in \mathcal{B}_1(\mathcal{H}),\\
\det_{\mathcal{H}}(I + T_1T_2) &= \det_{\mathcal{H}}(I + T_2T_1),\ \ T_1, T_2 \in \mathcal{B}(\mathcal{H}), && T_1T_2, T_2T_1 \in \mathcal{B}_1(\mathcal{H}).
\end{aligned}$$

In the following, let H_0, H be self-adjoint operators in $\mathcal{H}$ with $\operatorname{dom}(H_0) = \operatorname{dom}(H)$, and let $V = H - H_0$. Assume that $VR_z(H_0) \in \mathcal{B}_1(\mathcal{H})$, where $R_z(T)$ denotes the resolvent of an operator T, that is, $R_z(T) = (T - zI)^{-1}$. Under these assumptions one can introduce the *perturbation determinant*

$$\begin{aligned}
\Delta(z) = \Delta_{H/H_0}(z) :=\ &\det_{\mathcal{H}}(I + VR_z(H_0))\\
=\ &\det_{\mathcal{H}}\big((H - zI)(H_0 - zI)^{-1}\big), \quad \operatorname{Im}(z) \neq 0.
\end{aligned}$$

Next we briefly recall some properties of perturbation determinants.

For self-adjoint operators H_0, H the mapping $z \to \Delta_{H/H_0}(z)$ is analytic in both the half-planes $\mathrm{Im}(z) > 0$ and $\mathrm{Im}(z) < 0$ and

$$\Delta_{H/H_0}(\bar{z}) = \overline{\Delta_{H/H_0}(z)}, \quad \mathrm{Im}(z) \neq 0.$$

One has $\Delta_{H/H_0}(z) \neq 0$ for $\mathrm{Im}(z) \neq 0$.

In addition, since $V \in \mathcal{B}_1(\mathcal{H})$, standard properties of resolvents imply that

$$\|V R_{H_0}(z)\|_1 \to 0 \text{ as } |\mathrm{Im}(z)| \to \infty,$$

and therefore,

$$\Delta_{H/H_0}(z) \to 1 \text{ as } |\mathrm{Im}(z)| \to \infty.$$

Since the function $\Delta_{H/H_0}(\cdot)$ is analytic in the open upper and lower half-plane and since $\Delta_{H/H_0}(z) \neq 0$, $\mathrm{Im}(z) \neq 0$, it is a standard fact from complex analysis that there exists a function $G(\cdot)$ analytic in both of the upper and lower half-planes such that $e^G = \Delta_{H/H_0}$. Naturally, one denotes the function G by $\ln(\Delta_{H/H_0})$. It is clear that the function $\ln(\Delta_{H/H_0})$ is multivalued and its different values at a point z, $\mathrm{Im}(z) \neq 0$, differ by $2\pi i k$, $k \in \mathbb{Z}$. Since $\Delta_{H/H_0}(z) \to 1$, as $|\mathrm{Im}(z)| \to \infty$, one *fixes the branch* of the function $\ln(\Delta_{H/H_0})$ by requiring that $\ln(\Delta_{H/H_0}(z)) \to 0$ as $|\mathrm{Im}(z)| \to \infty$.

2.2. Construction of the SSF due to M.G. Krein

To construct the spectral shift function by Krein's method we exploit the following representation of the function $\ln(\Delta_{H/H_0}(z))$,

$$\ln(\Delta_{H/H_0}(z)) = \int_{\mathbb{R}} \frac{\xi(\lambda; H, H_0)\, d\lambda}{\lambda - z}, \quad \mathrm{Im}(z) \neq 0, \tag{2.2}$$

with a real-valued $\xi(\,\cdot\,; H, H_0) \in L_1(\mathbb{R})$, where $L_1(\mathbb{R})$ denotes the space of all (Lebesgue) integrable functions on $\mathbb{R}$.

The proof of (2.2) relies on the following classical result from complex analysis.

Theorem 2.1 (Privalov representation theorem). *Suppose that F is holomorphic in the open upper half-plane. If $\mathrm{Im}(F)$ is bounded and non-negative (respectively, non-positive) and if $\sup_{y \geqslant 1} y|F(iy)| < \infty$, then there exists a non-negative (respectively, non-positive) real-valued function $\xi \in L_1(\mathbb{R})$ such that*

$$F(z) = \int_{\mathbb{R}} \frac{\xi(\lambda)\, d\lambda}{z - \lambda}, \quad \mathrm{Im}(z) > 0.$$

The function ξ is uniquely determined by the Stieltjes inversion formula,

$$\xi(\lambda) = \frac{1}{\pi} \lim_{\varepsilon \downarrow 0+} \mathrm{Im}(F(\lambda + i\varepsilon)) \text{ for a.e. } \lambda \in \mathbb{R}.$$

Next we sketch the proof of the first theorem of Krein (see Theorem 2.2).

To verify the assumptions in Privalov's Theorem for $F = \ln(\Delta_{H/H_0})$, Krein proceeded as follows:

- First, suppose that $\operatorname{rank}(V) = 1$, that is, $V = \gamma(\cdot, h)h, \quad h \in \mathcal{H}, \quad \|h\| = 1$, $\gamma \in \mathbb{R}$. Then
$$\Delta_{H/H_0}(z) = 1 + \gamma(R_{H_0}(z)h, h).$$
Using this explicit form of the perturbation determinant one can prove that the function $\ln(\Delta_{H/H_0}(\cdot))$ satisfies all the assumptions in Privalov's theorem (for details see, e.g., Yafaev's book [62]). Hence, there exists a function $\xi(\lambda; H, H_0)$ satisfying (2.2), and furthermore, the function $\xi(\,\cdot\,; H, H_0)$ can be expressed in the form
$$\xi(\lambda; H, H_0) = \frac{1}{\pi} \lim_{\varepsilon \to +0} \operatorname{Im}(\ln(\Delta_{H/H_0}(\lambda + i\varepsilon))), \quad \text{a.e. } \lambda \in \mathbb{R}. \tag{2.3}$$
- Suppose now, that $\operatorname{rank}(V) = n < \infty$, that is,
$$V = \sum_{k=1}^{n} \gamma_k(\cdot, h_k)h_k, \quad \gamma_k = \bar{\gamma}_k,\ \|h_k\| = 1,\ 1 \leqslant k \leqslant n.$$
Denoting
$$V_m = \sum_{k=1}^{m} \gamma_k(\cdot, h_k)h_k, \quad H_m = H_0 + V_m, \quad 1 \leqslant m \leqslant \operatorname{rank}(V),$$
one infers that the difference $H_m - H_{m-1}$ is a rank-one operator. In addition, by the multiplicative property of the determinant one concludes that
$$\ln(\Delta_{H/H_0}(z)) = \sum_{m=1}^{n} \ln(\Delta_{H_m/H_{m-1}}(z)). \tag{2.4}$$
Applying the first step to the operators H_m, H_{m-1} one infers the existence of the corresponding SSFs $\xi(\,\cdot\,; H_m, H_{m-1})$, $1 \leqslant m \leqslant \operatorname{rank}(V)$.
Set
$$\xi(\lambda; H, H_0) = \sum_{m=1}^{n} \xi(\lambda; H_m, H_{m-1}), \quad 1 \leqslant k \leqslant n.$$

There are $L_1(\mathbb{R})$-norm estimates for each $\xi(\,\cdot\,; H_m, H_{m-1})$ which ensure that the function $\xi(\lambda; H, H_0)$ is integrable. Furthermore, since for every m, the representations (2.2) and (2.3) for $\ln(\Delta_{H_m/H_{m-1}})$ and $\xi(\lambda; H_m, H_{m-1})$, respectively, hold, one can infer from (2.4) and the definition of $\xi(\lambda; H, H_0)$ that representations (2.2) and (2.3) hold also for $\ln(\Delta_{H/H_0})$ and $\xi(\lambda; H, H_0)$.

- Suppose now, that V is an arbitrary trace class perturbation. Let V_n be a sequence of finite-rank operators, such that $\|V - V_n\|_1 \to 0$, $n \to \infty$. Set
$$\xi(\lambda; H, H_0) = \sum_{n} \xi(\lambda; H_n, H_{n-1}),$$
where the sum now is infinite (unless, V is a finite-rank operator).
Then, convergence properties of determinants and the $L_1(\mathbb{R})$-norm estimate for each $\xi(\,\cdot\,; H_n, H_{n-1})$ imply that this series converges in $L_1(\mathbb{R})$ and all the desired representations (2.2) and (2.3) for $\ln(\Delta_{H/H_0})$ and $\xi(\,\cdot\,; H, H_0)$ hold.

The following result is the first theorem of M.G. Krein.

Theorem 2.2 ([43]). *Let $V \in \mathcal{B}_1(\mathcal{H})$ be self-adjoint. Then the following representation holds:*

$$\ln(\Delta_{H/H_0}(z)) = \int_{\mathbb{R}} \frac{\xi(\lambda; H, H_0)\, d\lambda}{\lambda - z}, \quad \operatorname{Im}(z) \neq 0,$$

where

$$\xi(\lambda; H, H_0) = \frac{1}{\pi} \lim_{\varepsilon \downarrow 0} \operatorname{Im}(\ln(\Delta_{H/H_0}(\lambda + i\varepsilon))) \text{ for a.e. } \lambda \in \mathbb{R}, \tag{2.5}$$

in particular, the limit in (2.5) *exists for a.e.* $\lambda \in \mathbb{R}$. *In addition,*

$$\int_{\mathbb{R}} |\xi(\lambda; H, H_0)|\, d\lambda \leqslant \|V\|_1, \quad \int_{\mathbb{R}} \xi(\lambda; H, H_0)\, d\lambda = \operatorname{tr}_{\mathcal{H}}(V). \tag{2.6}$$

Moreover, $\xi(\lambda; H, H_0) \leqslant k_+$ (*respectively,* $\xi(\lambda; H, H_0) \geqslant -k_-$) *for a.e.* $\lambda \in \mathbb{R}$, *provided that the perturbation* V *has only* k_+ *positive* (*respectively,* k_- *negative*) *eigenvalues.*

Next, we turn to the rigorously proved trace formula, which is now customarily referred to the Lifshitz–Krein trace formula.

Theorem 2.3 (Second theorem of M.G. Krein). *Let $V \in \mathcal{B}_1(\mathcal{H})$ and assume that $f \in C^1(\mathbb{R})$ and its derivative admits the representation*

$$f'(\lambda) = \int_{\mathbb{R}} \exp(-i\lambda t)\, dm(t), \quad |m|(\mathbb{R}) < \infty,$$

for a finite (*complex*) *measure* m. *Then* $[f(H) - f(H_0)] \in \mathcal{B}_1(\mathcal{H})$, *and the following trace formula holds:*

$$\operatorname{tr}_{\mathcal{H}}(f(H) - f(H_0)) = \int_{\mathbb{R}} f'(\lambda)\xi(\lambda; H, H_0)\, d\lambda. \tag{2.7}$$

Remark 2.4.

(i) As is clearly seen from the arguments sketched, Krein's original proof was based on complex analysis. Attempts to produce a "real-analytic proof" are discussed later.

(ii) The function $\xi(\,\cdot\,; H, H_0)$ is an element of $L_1(\mathbb{R})$, that is, it represents an *equivalence class* of Lebesgue measurable functions. Therefore, generally speaking, the notation $\xi(\lambda; H, H_0)$ is meaningless for a fixed $\lambda \in \mathbb{R}$.

(iii) For a trace class perturbation V, the spectral shift function $\xi(\,\cdot\,; H, H_0)$ is *unique.*

(iv) The Lifshitz–Krein trace formula can be extended in various ways. One could attempt to describe the class of functions f, for which this formula holds; however, we will not cover this direction. Another important direction is to enlarge the class of perturbations $H - H_0$. We shall present some results in this direction below. ◇

2.3. Properties of the spectral shift function

Let H_0, H_1 and H be such that $(H_1 - H_0), (H - H_1) \in \mathcal{B}_1(\mathcal{H})$. First, we will list the simplest properties of the SSF.

These are that for a.e. $\lambda \in \mathbb{R}$ we have

$$\xi(\lambda; H, H_1) + \xi(\lambda; H_1, H_0) = \xi(\lambda; H, H_0),$$

in particular, $\xi(\lambda; H, H_0) = -\xi(\lambda; H_0, H)$, and also the inequality

$$\|\xi(\,\cdot\,; H, H_0) - \xi(\,\cdot\,; H_1, H_0)\|_1 \leqslant \|H - H_1\|_1$$

holds. In addition, if $H \geqslant H_1$, then

$$\xi(\lambda; H, H_0) \geqslant \xi(\lambda; H_1, H_0) \text{ for a.e. } \lambda \in \mathbb{R}.$$

Next, we describe some special situations where one can select concrete representatives from the equivalence class $\xi(\,\cdot\,; H, H_0)$, which justifies the term "the spectral shift function". These properties of the SSF $\xi(\,\cdot\,; H, H_0)$ are associated with the spectra of the operators H_0 and H. For the complete proof we refer to [62, Ch. 8]

(i) Let δ be an interval (possibly unbounded) such that $\delta \subset \rho(H_0) \cap \rho(H)$. Then $\xi(\,\cdot\,; H, H_0)$ takes a *constant integer value* on δ, that is,

$$\xi(\lambda; H, H_0) = n, \quad n \in \mathbb{Z},\ \lambda \in \delta.$$

If the interval δ contains a half-line, then the integrability condition on $\xi(\,\cdot\, H, H_0)$ implies that $n = 0$.

(ii) Let μ be an isolated eigenvalue of multiplicity $\alpha_0 < \infty$ of H_0 and multiplicity α for H. Then

$$\xi(\mu_+; H, H_0) - \xi(\mu_-; H, H_0) = \alpha_0 - \alpha. \tag{2.8}$$

Property (ii) can be generalized as follows:

(iii) Suppose that in some interval (a_0, b_0) the spectrum of H_0 is discrete (i.e., the spectrum of H_0 consists at most of eigenvalues of H_0 of *finite* multiplicity all of which are *isolated* points of $\sigma(H_0)$). Then, by Weyl's theorem on the invariance of essential spectra (see, e.g., [38, Theorem 5.35]), H has discrete spectrum in (a_0, b_0) as well.

Let $\delta = (a, b)$, $a_0 < a < b < b_0$. Introduce the *eigenvalue counting functions* $N_0(\delta)$ and $N(\delta)$ of the operators H_0 and H, respectively, in the interval δ as the sum of the multiplicities of the eigenvalues in δ of the operator H_0, respectively, H. Since the interval δ is finite and both operators H_0, H have discrete spectrum, $N_0(\delta)$ and $N(\delta)$ are finite. In this case one has the equality,

$$\xi(b_-; H, H_0) - \xi(a_+; H, H_0) = N_0(\delta) - N(\delta). \tag{2.9}$$

The preceding property implies, in particular, the following fact.

(iv) Let H_0 be a non-negative self-adjoint operator with purely discrete spectrum (i.e., $\sigma_{\mathrm{ess}}(H_0) = \emptyset$). Since the perturbation V is trace class, there exists $c \in \mathbb{R}$, such that $H \geqslant c$, that is, H is also lower semibounded. Generally, H will of course not be non-negative and so one should expect negative eigenvalues of H. Thus, property (iii) implies that for $\lambda < 0$,

$$\xi(\lambda_-) = -N(\lambda, H),$$

where $N(\lambda, H)$ is the sum of multiplicities of the eigenvalues of H lying to the left of the point $\lambda < 0$.

On the other hand, the following result demonstrates that any function from $L_1(\mathbb{R})$ arises as the spectral shift function for some pair of operators.

(v) Let ξ be an arbitrary real-valued element of $L_1(\mathbb{R})$. Then, there exists a pair of self-adjoint operators H_0, H, such that $(H - H_0) \in \mathcal{B}_1(\mathcal{H})$ and ξ is the SSF $\xi(\,\cdot\,; H, H_0)$ for the pair (H, H_0). In addition, if $0 \leqslant \xi \leqslant 1$, then there is a pair H_0, H such that $H - H_0$ is a positive rank-one operator [43], [45].

2.4. Earlier real-analytic approaches

In the following we discuss other approaches for constructing the SSF. The first attempt to prove the existence of the SSF without relying on complex analysis was made by Birman and Solomyak in [11]. This method is based on consideration of the *family of operators*,

$$H_s = H_0 + sV, \quad s \in [0,1], \quad H = H_1,$$

and their family of spectral measures $\{E_{H_s}(\lambda)\}_{\lambda\in\mathbb{R}}$. Employing the *theory of double operator integrals* also developed by these authors, it can be proved that for a sufficiently large class of functions f, there exists a continuous derivative in $\mathcal{B}_1(\mathcal{H})$-norm of the operator-valued function $s \mapsto f(H_s)$, represented in the double operator integral form as

$$\frac{df(H_s)}{ds} = \int_{\mathbb{R}}\int_{\mathbb{R}} \frac{f(\mu) - f(\lambda)}{\mu - \lambda}\, dE_{H_s}(\mu) V dE_{H_s}(\lambda).$$

Furthermore, Birman and Solomyak obtained the equality

$$\operatorname{tr}_{\mathcal{H}}\left(\frac{df(H_s)}{ds}\right) = \int_{\mathbb{R}} f'(\lambda)\, d\operatorname{tr}(VE_{H_s}(\lambda)).$$

Integration with respect to s then yields the formula

$$\operatorname{tr}_{\mathcal{H}}(f(H) - f(H_0)) = \int_{\mathbb{R}} f'(\lambda)\, d\Xi_{H,H_0}(\lambda),$$

where the *spectral averaging measure* Ξ_{H,H_0} is defined by

$$\Xi_{H,H_0}(X) = \int_0^1 \operatorname{tr}(VE_{H_s}(X))\, ds,$$

with $X \subseteq \mathbb{R}$ a Borel set.

However, this attempt to yield an alternative proof of Krein's Theorem 2.3 was unsuccessful since the authors failed to establish the absolute continuity of the latter measure with respect to Lebesgue measure.

We note, that *if* one introduces $\xi(\cdot; H, H_0)$ by Krein's Theorem 2.2, then

$$\int_X \xi(\lambda; H, H_0)\, d\lambda = \Xi_{H,H_0}(X),$$

for any Borel set $X \subseteq \mathbb{R}$, that is, the measure Ξ is indeed absolutely continuous.

The second attempt to deliver a real-analytic proof was due to Voiculescu [60], his method was based on the classical Weyl–Berg–von Neumann theorem. However, his attempt also failed to recover the full generality of Krein's original result.

Another attempt to obtain a proof of Krein's formula without appealing to complex-analytic methods was introduced by Sinha and Mohapatra [57]. Again, that attempt did not yield the full generality of the result and does not seem to apply to general semifinite von Neumann algebras.

2.5. The case of semifinite von Neumann algebras

Some problems in noncommutative geometry require replacing the algebra $\mathcal{B}(\mathcal{H})$ of all bounded linear operators on a Hilbert space $\mathcal{H}$ and unbounded operators on $\mathcal{H}$ with a general semifinite von Neumann algebra $\mathcal{M}$ and unbounded operators affiliated with $\mathcal{M}$. A typical example of differential operators affiliated to semifinite von Neumann algebras arises in the context of Atiyah's L^2-index theorem and its extensions. (For example, the paper [13] considers the case of lifts of Dirac-type operators acting on sections of a finite-dimensional vector bundle over a complete Riemannian manifold M to a Galois cover $\widetilde{M}$ of M.)

The first attempt to extend Krein's results and methods to the realm of semifinite von Neumann algebras was made in [10]. It broadly followed Krein's complex analysis proof. However, it does not offer an adequate extension to general semifinite von Neumann algebras of the notion of the perturbation determinant, which plays the key role in Krein's proof. This difficulty is circumvented in [10] via the use of the notion of a *Brown measure* [14].

The core of the approach in [10] is to show that there exists a neighbourhood of the spectrum of the operator $R_z(H_0)V$, which does not intersect the half-line $(-\infty, -1]$, in the case where $V \geqslant 0$ or $-V \geqslant 0$. One then applies one of the principal results of Brown [14] to establish estimates needed for the application of the Privalov representation theorem (see Theorem 2.1). Finally, the proof in [10] proceeded under the additional assumption that $H - H_0$ is a bounded operator belonging to the space $\mathcal{L}_1(\mathcal{M}, \tau)$, the predual of the algebra $\mathcal{M}$.

Another subsequent paper [9] employed the double operator integral (DOI) technique due to Birman and Solomyak, but in a slightly different form suitable for semifinite von Neumann algebras using an approach from [8]. Following the idea of Birman and Solomyak, one can define the spectral shift measure for a pair (H, H_0), by setting

$$\Xi_{H,H_0}(X) = \int_0^1 \tau(V E_{H_s}(X)) ds,$$

where τ is a faithful normal semifinite trace on $\mathcal{M}$. Assuming that H_0 has τ-*compact resolvent*, and the perturbation V is *bounded*, it can be proved that the spectral shift measure Ξ_{H,H_0} is *absolutely continuous* with respect to the Lebesgue measure and the resulting Radon–Nikodym derivative is the SSF for the pair (H, H_0).

The first complete "real analytic proof" of the Lifshitz–Krein formula is due to Potapov, Sukochev, and Zanin [53]. That paper delivers a rather short and straightforward proof of the Lifshitz–Krein formula without any use of complex analytic tools. The approach in [53] can be characterized as a combination of methods drawn from the double operator integration theory of Birman and Solomyak and from Voiculescu's ideas based on the Weyl–Berg–von Neumann theorem. The result holds for an arbitrary semifinite von Neumann algebra $\mathcal{M}$, equipped with a faithful normal semifinite trace τ and (unbounded) operators H_0, H affiliated with $\mathcal{M}$, such that $H - H_0$ belongs to the space $\mathcal{L}_1(\mathcal{M}, \tau)$.

We denote by W_1 the class of all differentiable functions $f : \mathbb{R} \to \mathbb{R}$ such that $\mathcal{F}(f') \in L_1(\mathbb{R})$, where the symbol $\mathcal{F}$ denotes the standard Fourier transform. The following theorem is the main result of [53]:

Theorem 2.5. *Let $\mathcal{M}$ be a von Neumann algebra equipped with a faithful normal semifinite trace τ. If the self-adjoint operators H_0, H affiliated with $\mathcal{M}$ are such that $(H - H_0) \in \mathcal{L}_1(\mathcal{M}, \tau)$, then there is a function $\xi(\,\cdot\,; H, H_0) \in L_1(\mathbb{R})$ such that the trace formula*

$$\tau(f(H) - f(H_0)) = \int_{\mathbb{R}} f'(\lambda)\, \xi(\lambda; H, H_0)\, d\lambda \tag{2.10}$$

holds for all $f \in W_1$.

Remark 2.6. If the von Neumann algebra $\mathcal{M}$ is the type I factor $\mathcal{B}(\mathcal{H})$ with the standard trace, then Theorem 2.5 delivers an alternative proof of Krein's result (i.e., Theorem 2.3). ◇

Below we outline the proof of Theorem 2.5.

We start by introducing the *distribution function* N_{H_0} of the operator H_0, that is,

$$N_{H_0}(t) := \tau(E_{H_0}(t, \infty)), \quad t \geqslant 0,$$

where $E_{H_0}((t, \infty))$ is the spectral projection of the self-adjoint operator H_0 corresponding to the interval (t, ∞).

The proof in [53] is divided into several stages. For simplicity we denote by $\xi^{(j)}(\,\cdot\,; H, H_0)$ the function constructed on the jth step.

Step (i). Let the trace τ be *finite*, that is, $\tau(I) < \infty$ and $H_0, H \in \mathcal{M}$. In this case, the SSF is merely defined as

$$\xi^{(1)}(\,\cdot\,; H, H_0) = N_H(\cdot) - N_{H_0}(\cdot).$$

Since the trace τ is finite, both N_H and N_{H_0} are finite.

One should note the similarity of this formula with property (iii) of the SSF (see (2.9)). One can think of this equation as the "naive" definition of the SSF.

However, while this definition is correct for finite von Neumann algebras, there are examples of self-adjoint operators H, H_0 in infinite-dimensional Hilbert spaces with $H - H_0$ being a rank-one operator such that the operator $E_{H_0}((t,\infty)) - E_H((t,\infty))$ *is not* a trace class operator for all t on the spectrum [43] (the example concerns self-adjoint resolvents of Dirichlet and Neumann Laplacians on a half-line).

The function $\xi^{(1)}(\,\cdot\,; H, H_0)$ is supported on the interval $[-a, a]$, where $a := \max\{\|H_0\|_\infty, \|H\|_\infty\}$. Furthermore, it possesses a property similar to that of the Krein SSF (see (2.6)),

$$\|N_H - N_{H_0}\|_\infty \leqslant \tau(\operatorname{supp}(H - H_0)), \quad \|N_H - N_{H_0}\|_1 \leqslant \|H - H_0\|_1. \tag{2.11}$$

Step (ii). In the second step, the trace formula is proved for *bounded* operators $H_0, H \in \mathcal{M}$, with the perturbation $V = H - H_0$ being a *non-negative* operator with *τ-finite support*, and for functions of the form $f(s) = s^m$. Here we use an idea noted by Voiculescu, who proved the Krein trace formula for the case of polynomials.

Proving a result similar to the classical Berg–Weyl–von Neumann theorem we construct a family of τ-finite projections p_n, $n \in \mathbb{N}$, with $p_n \uparrow I$ such that

$$\tau((p_n H p_n)^m - (p_n H_0 p_n)^m) - \tau(H^m - H_0^m) \to 0 \text{ as } n \to \infty. \tag{2.12}$$

Since for every $n \in \mathbb{N}$, $\tau(p_n 1 p_n) < \infty$, by Step (i), there exists a positive function $\xi_n^{(1)} = \xi^{(1)}(\,\cdot\,; p_n H p_n, p_n H_0 p_n)$, supported on $[-a, a]$, satisfying the trace formula. In addition, by (2.11), the sequence $\{\xi_n^{(1)}\}_{n\in\mathbb{N}}$ is bounded in $L_\infty((-a, a))$. By the Banach–Alaoglu Theorem the latter is compact in the weak*-topology, and therefore, there exists a directed set $\mathbb{J}$ and a mapping $\psi : \mathbb{J} \to \mathbb{N}$ such that for every $n \in \mathbb{N}$, there exists $j(n) \in \mathbb{J}$ such that $\psi(j) > n$ for $j > j(n)$ and such that the net $\xi_{\psi(j)}^{(1)}(\,\cdot\,; p_{\psi(j)} H p_{\psi(j)}, p_{\psi(j)} H_0 p_{\psi(j)})$ converges in weak*-topology. The function $\xi^{(2)}(\,\cdot\; H, H_0)$ is then defined by

$$\xi^{(2)}(\,\cdot\,; H, H_0) := \lim_{j\in\mathbb{I}} \xi_{\psi(j)}^{(1)}(\,\cdot\,; p_{\psi(j)} H p_{\psi(j)}, p_{\psi(j)} H_0 p_{\psi(j)}),$$

and proved to be the SSF.

Step (iii). Let $H, H_0 \in \mathcal{M}$, $f \in C_b^2(\mathbb{R})$. In this step the assumptions $H \geqslant H_0$ and $\tau(\operatorname{supp}(H - H_0)) < \infty$ are removed.

It is proved that, without loss of generality, one can assume that $H \geqslant H_0$. Let $0 \leqslant D_n \leqslant H - H_0$, $n \in \mathbb{N}$, be such that $D_n \uparrow H - H_0$ as $n \to \infty$, and $\tau(\operatorname{supp}(D_n)) < \infty$, $n \in \mathbb{N}$.

Since polynomials are dense in $C^2([-a, a])$, it follows from Step (ii) and DOI techniques that

$$\tau(f(H_0 + D_n) - f(H_0)) = \int_{-a}^{a} f'(\lambda) \xi^{(2)}(\lambda; H_0 + D_n, H_0)\, d\lambda, \quad f \in C_b^2(\mathbb{R}). \tag{2.13}$$

Then, proving that the sequence $\{\xi^{(2)}(\,\cdot\,; H_0 + D_n, H_0)\}_{n\in\mathbb{N}}$ increases and is uniformly bounded, one infers from the Monotone Convergence Principle that the sequence $\{\xi^{(2)}(\,\cdot\,; H_0 + D_n, H_0)\}_{n\in\mathbb{N}}$ converges in $L^1(\mathbb{R})$; its limit is denoted by $\xi^{(3)}(\,\cdot\,; H, H_0)$. This function is now the SSF for the pair (H, H_0).

Step (iv). The final step in this approach consists in removing the assumption that the operators H_0 and H are bounded. This is the key point of the proof in which DOI techniques are used in its full strength. This part of the proof is rather technical. We briefly outline the main ideas.

Choose a C^2-bijection $h : \mathbb{R} \to (a, b)$ for some $a, b \in \mathbb{R}$, $a < b$. Then the operators $h(H_0)$ and $h(H)$ are bounded, so that applying Step (iii) to the operators $h(H_0)$ and $h(H)$, one defines

$$\xi^{(4)}(\,\cdot\,; H, H_0) := \xi^{(3)}(\,\cdot\,; h(H), h(H_0)) \circ h.$$

Next, employing again DOI techniques, one proves that this definition of the SSF *does not depend* on the function h and, moreover,

(α) if $H \geqslant H_0$, then $\xi^{(4)}(\,\cdot\,; H, H_0) \geqslant 0$,
(β) $\xi^{(4)}(\,\cdot\,; H, H_0) \in L_1(\mathbb{R})$.

2.6. More general classes of perturbations

At this point we return to the case where the von Neumann algebra is the algebra $\mathcal{B}(\mathcal{H})$ equipped with the standard trace and consider the situation when the perturbation is no longer a trace class operator. We note, that for the following results we *will not specify* the class of functions f, for which the Krein trace formula holds. We are only interested in the *existence* of the SSF for a more general class of perturbations.

The first result, generalizing the class of operators H_0, H is due to M.G. Krein [44].

Theorem 2.7 (Resolvent comparable case). *Let the self-adjoint operators H_0, H be such that*

$$[R_H(z) - R_{H_0}(z)] \in \mathcal{B}_1(\mathcal{H}), \quad z \in \rho(H_0) \cap \rho(H). \tag{2.14}$$

Then there exists a spectral shift function $\xi(\,\cdot\,; H, H_0)$, satisfying the weighted integrability condition

$$\xi(\lambda; H, H_0) \in L^1\big(\mathbb{R}; (1 + \lambda^2)^{-1} d\lambda\big).$$

We emphasize that in the present resolvent comparable case (2.14), this SSF is defined only *up to an additive constant.*

Just as in the case of a trace class perturbation, the SSF for resolvent comparable operators H_0, H possesses the following property:

- Suppose that in some interval (a_0, b_0) the spectrum of H_0 is *discrete* and let $\delta = (a, b)$, $a_0 < a < b < b_0$. Then the analogue of (2.9) holds, that is,

$$\xi(b_-; H, H_0) - \xi(a_+; H, H_0) = N_0(\delta) - N(\delta), \tag{2.15}$$

  where $N_0(\delta)$ (respectively, $N(\delta)$) are the sum of the multiplicities of the eigenvalues of H_0 (respectively, H) in δ.

In the particular case of *lower semibounded operators* H_0 and H equality (2.15) allows us to *naturally fix* the additive constant in the following way. To the left of the spectra of H_0 and H, the eigenvalue counting functions $N_0(\cdot)$ and $N(\cdot)$ are zero. Therefore, by equality (2.15) the SSF $\xi(\,\cdot\,;H,H_0)$ is a constant to the left of the spectra of H_0 and H, and it is custom to set this constant equal to zero,

$$\xi(\lambda;H,H_0)=0, \quad \lambda<\inf(\sigma(H_0)\cup\sigma(H)).$$

In the following we describe a particular way to introduce the SSF for the pair (H,H_0) by what is usually called the *invariance principle*. We note that this principle was used in a construction in [53] of the SSF for trace class perturbations at Step (iv), where we passed to unbounded operators.

Let Ω be an interval containing the spectra of H_0 and H, and let ϕ be an arbitrary bounded monotone "sufficiently" smooth function on Ω. Suppose that

$$[\phi(H)-\phi(H_0)]\in\mathcal{B}_1(\mathcal{H})$$

then, the SSF $\xi(\,\cdot\,;H,H_0)$ can be defined as follows:

$$\xi(\lambda;H,H_0)=\operatorname{sgn}\big(\phi'(\lambda)\big)\xi(\phi(\lambda);\phi(H),\phi(H_0)). \tag{2.16}$$

For the function $\xi(\,\cdot\,;H,H_0)$ the Lifshitz–Krein trace formula (2.7) holds for some class of admissible functions f. The latter class depends on ϕ.

We note the following result (see [62, Sect. 8.11]):

Proposition 2.8. *Let* $(H-H_0)\in\mathcal{B}_1(\mathcal{H})$. *Then the spectral shift functions for the pairs* (H,H_0) *and* $(\phi(H),\phi(H_0))$ *are associated via equality* (2.16) *up to an additive, integer-valued constant.*

The methods of construction of the SSF introduced in this survey are only a sample of a plethora of possibilities. There are many others, which we did not cover here. We only mention a few of them:

- Sobolev [58] suggested a way of constructing the SSF for trace class perturbations via the "argument of the perturbation determinant". This construction allows one to establish *pointwise* estimates on the SSF, and, in some cases, proves continuity of SSF on the absolutely continuous spectrum of H_0 (the latter coincides with that of H).
- Koplienko [40] proved the existence of the SSF for the pair of operators (H,H_0) under the assumption that for some $\varepsilon>0, 1\leqslant p<\infty$,
$$[R_H(z)-R_{H_0}(z)](H_0^2+i)^{-\varepsilon}\in\mathcal{B}_1(\mathcal{H}), \quad [R_H(z)-R_{H_0}(z)]\in\mathcal{B}_p(\mathcal{H}),$$
where $\mathcal{B}_p(\mathcal{H})$ denotes the Schatten–von Neumann ideal in $\mathcal{B}(\mathcal{H})$.
- Yafaev [63] proved that the SSF exists for a pair of operators H_0 and H satisfying the assumption that for some $m\in\mathbb{N}$, m odd,
$$\big[R_H^m(z)-R_{H_0}^m(z)\big]\in\mathcal{B}_1(\mathcal{H}).$$
- Koplienko [39] proposed another function, which is called the Koplienko SSF [39], and is constructed under the assumption that $(H-H_0)\in\mathcal{B}_2(\mathcal{H})$ (see also [31]). For recent developments of this line of thought, we refer to [52].

3. The Witten index

The Witten index of an operator T in a complex separable Hilbert space $\mathcal{H}$ provides a generalisation of the Fredholm index of T in certain cases where the operator T ceases to have the Fredholm property. The Witten index possesses stability properties with respect to additive perturbations, which are analogous to, but more restrictive than, the stability properties of the Fredholm index (roughly speaking, only relative trace class perturbations, as opposed to relative compact ones, are permitted). After the publication of [61] this notion became popular in connection with a variety of examples in supersymmetric quantum theory in the 1980s. One reason the Witten index has attracted little attention in recent years is that its connection with geometric questions remains unclear (see however [16], [22]). This is a matter deserving further investigation. For more historical details we refer to the paragraphs following Theorem 3.3.

First, we recall the definitions and some of the basic properties of the Witten index. In the next section, we will derive new properties of the Witten index of a certain model operator.

We start with the following facts on trace class properties of resolvent and semigroup differences.

Then the following well-known and standard assertions hold for resolvent and semigroup comparable operators (see item (ii) below):

Proposition 3.1. *Suppose that $0 \leqslant S_j$, $j = 1, 2$, are nonnegative, self-adjoint operators in $\mathcal{H}$.*

(i) *If $\big[(S_2 - z_0)^{-1} - (S_1 - z_0)^{-1}\big] \in \mathcal{B}_1(\mathcal{H})$ for some $z_0 \in \rho(S_1) \cap \rho(S_2)$, then actually,*

$$\big[(S_2 - z)^{-1} - (S_1 - z)^{-1}\big] \in \mathcal{B}_1(\mathcal{H}) \text{ for all } z \in \rho(S_1) \cap \rho(S_2).$$

(ii) *If $\big[e^{-t_0 S_2} - e^{-t_0 S_1}\big] \in \mathcal{B}_1(\mathcal{H})$ for some $t_0 > 0$, then*

$$\big[e^{-tS_2} - e^{-tS_1}\big] \in \mathcal{B}_1(\mathcal{H}) \text{ for all } t \geqslant t_0.$$

The preceding fact allows one to consider the following two definitions.

Let T be a closed, linear, densely defined operator in $\mathcal{H}$. Suppose that for some (and hence for all) $z \in \mathbb{C}\backslash[0, \infty) \subseteq \rho(T^*T) \cap \rho(TT^*)$,

$$\big[(T^*T - z)^{-1} - (TT^* - z)^{-1}\big] \in \mathcal{B}_1(\mathcal{H}).$$

Then one introduces the resolvent regularization

$$\Delta_r(T, \lambda) = (-\lambda)\,\mathrm{tr}_{\mathcal{H}}\big((T^*T - \lambda)^{-1} - (TT^* - \lambda)^{-1}\big), \quad \lambda < 0.$$

The resolvent regularized Witten index $W_r(T)$ of T is then defined by

$$W_r(T) = \lim_{\lambda \uparrow 0} \Delta_r(T, \lambda),$$

whenever this limit exists.

Similarly, suppose that for some $t_0 > 0$

$$\big[e^{-t_0 T^*T} - e^{-t_0 TT^*}\big] \in \mathcal{B}_1(\mathcal{H}).$$

Then $\big(e^{-tT^*T} - e^{-tTT^*}\big) \in \mathcal{B}_1(H)$ for all $t > t_0$ and one introduces the semigroup regularization

$$\Delta_s(T,t) = \operatorname{tr}_{\mathcal{H}}\big(e^{-tT^*T} - e^{-tTT^*}\big), \quad t > 0.$$

The semigroup regularized Witten index $W_s(T)$ of T is then defined by

$$W_s(T) = \lim_{t\uparrow\infty} \Delta_s(T,t),$$

whenever this limit exists.

One recalls that a densely defined and closed operator T in a Hilbert space $\mathcal{H}$ is said to be *Fredholm* if $\operatorname{ran}(T)$ is closed and $\dim(\ker(T)) + \dim(\ker(T^*)) < \infty$. In this case, the *Fredholm index* $\operatorname{ind}(T) := \dim(\ker(T)) - \dim(\ker(T^*))$. The following result, obtained in [15] and [32], states that both (resolvent and semigroup) regularized Witten indices coincide with the Fredholm index in the special case of Fredholm operators.

Theorem 3.2. *Let T be an (unbounded) Fredholm operator in H. Suppose that $\big[(T^*T-z)^{-1}-(TT^*-z)^{-1}\big]$, $\big[e^{-t_0T^*T}-e^{-t_0TT^*}\big] \in \mathcal{B}_1(\mathcal{H})$ for some $z \in \mathbb{C}\backslash[0,\infty)$, and $t_0 > 0$. Then*

$$\operatorname{ind}(T) = W_r(T) = W_s(T).$$

In general (i.e., if T is not Fredholm), $W_r(T)$ (respectively, $W_s(T)$) is not necessarily integer-valued; in fact, it can be any real number. As a concrete example, we mention the two-dimensional magnetic field system discussed by Aharonov and Casher [1] which demonstrates that the resolvent and semigroup regularized Witten indices have the meaning of (non-quantized) magnetic flux $F \in \mathbb{R}$ which indeed can be any prescribed real number.

Expressing the Witten index $W_s(T)$ (respectively, $W_r(T)$) of an operator T in terms of the spectral shift function $\xi(\,\cdot\,;T^*T,TT^*)$ requires of course the choice of a concrete representative of the SSF:

Theorem 3.3 ([15, 32]).

(i) *Suppose that*

$$\big[e^{-t_0T^*T} - e^{-t_0TT^*}\big] \in \mathcal{B}_1(\mathcal{H}),\ \ t_0 > 0 \ \text{ and the SSF } \xi(\,\cdot\,;T^*T,TT^*),$$

uniquely defined by the requirement $\xi(\lambda;T^*T,TT^*) = 0,\ \lambda < 0$, is continuous from above at $\lambda = 0$. Then the semigroup regularized Witten index $W_s(T)$ of T exists and

$$W_s(T) = -\xi(0_+;T^*T,TT^*).$$

(ii) *Suppose that $\big[(T^*T-z)^{-1}-(TT^*-z)^{-1}\big]$, $z\in\mathbb{C}\backslash[0,\infty)$ and $\xi(\cdot;T^*T,TT^*)$, uniquely defined by the requirement $\xi(\lambda;T^*T,TT^*) = 0,\ \lambda < 0$, is bounded and piecewise continuous on $\mathbb{R}$. Then the resolvent regularized Witten index $W_s(T)$ of T exists and*

$$W_r(T) = -\xi(0_+;T^*T,TT^*).$$

The first relations between index theory for not necessarily Fredholm operators and the Lifshitz–Krein spectral shift function were established in [15], [29], [32], and independently in [25]. In fact, inspired by index calculations of Callias [20] in connection with non-compact manifolds, the more general notion of the Witten index was studied and identified with the value of an appropriate spectral shift function at zero in [15] and [32] (see also [29], [59, Ch. 5]). Similiar investigations in search of an index theory for non-Fredholm operators were undertaken in [25] in a slightly different direction, based on principal functions and their connection to Krein's spectral shift function.

The index calculations by Callias created considerable interest, especially, in connection with certain aspects of supersymmetric quantum mechanics. Since a detailed list of references in this context is beyond the scope of this paper we only refer to [2], [3], [4], [5], [6], [12], [17], [19], [27], [28], [35], [36], [37], [41], [42], [49], [50], [59, Ch. 5] and the detailed lists of references cited therein. While [15] and [29] focused on index theorems for concrete one and two-dimensional supersymmetric systems (in particular, the trace formula (3.4) and the function $g_z(\cdot)$ in (3.3) were discussed in [15] and [29] in the special case where $\mathcal{H} = \mathbb{C}$), [32] treated abstract Fredholm and Witten indices in terms of the spectral shift function and proved their invariance with respect to appropriate classes of perturbations. Soon after, a general abstract approach to supersymmetric scattering theory involving the spectral shift function was developed in [16] (see also [18], [46, Chs. IX, X], [47]) and applied to relative index theorems in the context of manifolds Euclidean at infinity.

Example 3.4. As an example of practical use of the abstract results, [15] considered the operator

$$T = \frac{d}{dt} + M_\theta, \quad \operatorname{dom}(T) = W^{2,1}(\mathbb{R}),$$

acting on the standard Hilbert space $L^2(\mathbb{R})$. Here $W^{2,1}(\mathbb{R})$ is the Sobolev space, M_θ is the operator of multiplication by a bounded function θ on $\mathbb{R}$. Assuming existence of the asymptotes $\lim_{t\to\pm\infty} \theta(t) = \theta_\pm \in \mathbb{R}$, and some additional conditions on θ, it is shown in [15] that for the resolvent regularization one obtains

$$\begin{aligned} \Delta_r(T,\lambda) &= (-\lambda)\operatorname{tr}_{\mathcal{H}}\big((T^*T-\lambda)^{-1} - (TT^*-\lambda)^{-1}\big) \\ &= \big[\theta_+(\theta_+^2-\lambda)^{-1/2} + \theta_-(\theta_-^2-\lambda)^{-1/2}\big]/2, \quad \lambda \in \mathbb{C}\backslash[0,\infty), \end{aligned} \tag{3.1}$$

and therefore,

$$W_r(T) = [\operatorname{sgn}(\theta_+) - \operatorname{sgn}(\theta_-)]/2.$$

Next, we view the operator T from the preceding example as an operator of the form $T = \boldsymbol{D_A} = \frac{d}{dt} + \boldsymbol{A}$ on the Hilbert space $L^2(\mathbb{R};\mathbb{C})$, where $\boldsymbol{A}$ is the operator generated by the family of operators $\{A(t)\}_{t\in\mathbb{R}}$ on the Hilbert space $\mathbb{C}$, with $A(t)$ given by multiplication by $\theta(t)$, $t \in \mathbb{R}$.

Our main objective in this survey is to consider a more general situation where the family $\{A(t)\}$ consists of operators acting on an arbitrary complex, separable initial Hilbert space $\mathcal{H}$, and the resulting operator $\boldsymbol{D_A} = \frac{d}{dt} + \boldsymbol{A}$ acts on the Hilbert space $L^2(\mathbb{R};\mathcal{H})$. Operators of this form $\boldsymbol{D_A}$ arise in connection with Dirac-type operators (on compact and noncompact manifolds), the Maslov index, Morse theory (index), Floer homology, winding numbers, Sturm's oscillation theory, dynamical systems, etc. (cf. [30] and the extensive list of references therein).

To date, strong conditions need to be imposed on the family $A(t)$ in order to obtain the resolvent and semigroup Witten indices of $\boldsymbol{D_A}$ and express them in terms of the spectral shift function for the asymptotes $A_\pm$ of the family $A(t)$ as $t \to \pm\infty$. The following is the main hypothesis, under which the results stated below are proved.

Hypothesis 3.5.

(i) *Suppose $\mathcal{H}$ is a complex, separable Hilbert space.*

(ii) *Assume A_- is a self-adjoint operator on* $\operatorname{dom}(A_-) \subseteq \mathcal{H}$.

(iii) *Suppose there exists a family of bounded self-adjoint operators $B(t)$, $t \in \mathbb{R}$ with $t \mapsto B(t)$ weakly locally absolutely continuous on $\mathbb{R}$, implying the existence of a family of bounded self-adjoint operators $\{B'(t)\}_{t\in\mathbb{R}}$ in $\mathcal{H}$ such that for a.e. $t \in \mathbb{R}$,*

$$\frac{d}{dt}(g, B(t)h)_{\mathcal{H}} = (g, B'(t)h)_{\mathcal{H}}, \quad g, h \in \mathcal{H}.$$

(iv) *Assume that the family $\{B'(t)\}$ is A_-*-relative trace class*, that is, suppose that $B'(t)(|A_-|+1)^{-1} \in \mathcal{B}_1(\mathcal{H})$, $t \in \mathbb{R}$. In addition, we assume that*

$$\int_{\mathbb{R}} dt \, \big\| B'(t)(|A_-|+1)^{-1} \big\|_{\mathcal{B}_1(\mathcal{H})} < \infty.$$

Remark 3.6.

(i) We note that, in fact, the subsequent results hold in a more general situation, when the operators $B(t)$, $t \in \mathbb{R}$, are allowed to be unbounded and some additional measurability conditions of the families $\{B(t)\}$, $\{B'(t)\}$ are imposed.

(ii) The assumption (iv) above, that the operators $B'(t)$, $t \in \mathbb{R}$, are relative trace class, namely, $B'(t)(|A_-|+1)^{-1} \in \mathcal{B}_1(\mathcal{H})$, is the main assumption, which implies various trace relations below. In Section 5 we will discuss an example where we replace the relative trace class hypotheses with a relative Hilbert–Schmidt class assumption. ◇

From this point on we assume Hypothesis 3.5.

3.1. Definition of the operator $\boldsymbol{D_A}$

We introduce the family of self-adjoint operators $\{A(t)\}_{t\in\mathbb{R}}$ in $\mathcal{H}$ by

$$A(t) = A_- + B(t), \quad \operatorname{dom}(A(t)) = \operatorname{dom}(A_-), \ t \in \mathbb{R}.$$

Hypothesis 3.5 ensures the existence of the *asymptote* A_+ as $t \to \infty$ in the norm-resolvent sense, $\operatorname{dom}(A_+) = \operatorname{dom}(A_-)$, with A_+ self-adjoint in $\mathcal{H}$, that is

$$\lim_{t\to+\infty} \big\| (A(t) - z)^{-1} - (A_+ - z)^{-1} \big\|_{\mathcal{B}(H)} = 0.$$

Let $\boldsymbol{A}$ in $L^2(\mathbb{R};\mathcal{H})$ be the operator associated with the family $\{A(t)\}_{t\in\mathbb{R}}$ in $\mathcal{H}$ by

$$(\boldsymbol{A}f)(t) = A(t)f(t) \text{ for a.e. } t \in \mathbb{R},$$
$$f \in \operatorname{dom}(\boldsymbol{A}) = \bigg\{ g \in L^2(\mathbb{R};\mathcal{H}) \,\bigg|\, g(t) \in \operatorname{dom}(A(t)) \text{ for a.e. } t \in \mathbb{R},$$
$$t \mapsto A(t)g(t) \text{ is (weakly) measurable}, \int_{\mathbb{R}} dt\, \|A(t)g(t)\|_{\mathcal{H}}^2 < \infty \bigg\}.$$

We define also the operator $\mathbf{d/dt}$ in $L^2(\mathbb{R};\mathcal{H})$ by setting

$$\left(\frac{\mathbf{d}}{\mathbf{dt}}f\right)(t) = f'(t) \text{ a.e. } t \in \mathbb{R}, \quad f \in \operatorname{dom}(\mathbf{d/dt}) = W^{2,1}(\mathbb{R};\mathcal{H}),$$

where $W^{1,2}(\mathbb{R};\mathcal{H})$ denotes the usual Sobolev space of $L^2(\mathbb{R};\mathcal{H})$-functions with the first distributional derivative in $L^2(\mathbb{R};\mathcal{H})$.

Now, we introduce the operator $\boldsymbol{D_A}$ in $L^2(\mathbb{R};\mathcal{H})$ by setting

$$\boldsymbol{D_A} = \frac{\mathbf{d}}{\mathbf{dt}} + \boldsymbol{A}, \quad \operatorname{dom}(\boldsymbol{D_A}) = \operatorname{dom}(\mathbf{d/dt}) \cap \operatorname{dom}(\boldsymbol{A}). \tag{3.2}$$

Proposition 3.7. [30] *Assume Hypothesis* 3.5*. Then the operator* $\boldsymbol{D_A}$ *is densely defined and closed in* $L^2(\mathbb{R};\mathcal{H})$ *and the adjoint* $\boldsymbol{D_A^*}$ *of* $\boldsymbol{D_A}$ *in* $L^2(\mathbb{R};\mathcal{H})$ *is given by*

$$\boldsymbol{D_A^*} = -\frac{\mathbf{d}}{\mathbf{dt}} + \boldsymbol{A}, \quad \operatorname{dom}(\boldsymbol{D_A^*}) = \operatorname{dom}(\boldsymbol{D_A}).$$

3.2. The principle trace formula

The following result relates the trace of the difference of the resolvents of positive operators $|\boldsymbol{D_A}|^2$ and $|\boldsymbol{D_A^*}|^2$ in $L^2(\mathbb{R};\mathcal{H})$, and the trace of the difference of $g_z(A_+)$ and $g_z(A_-)$ in $\mathcal{H}$, where

$$g_z(x) = x(x^2 - z)^{-1/2}, \quad x \in \mathbb{R},\ z \in \mathbb{C}\backslash[0,\infty). \tag{3.3}$$

Theorem 3.8. *Assume Hypothesis* 3.5*. Then,*

$$\big[\big(|\boldsymbol{D_A^*}|^2 - z\big)^{-1} - \big(|\boldsymbol{D_A}|^2 - z\big)^{-1}\big] \in \mathcal{B}_1\big(L^2(\mathbb{R};\mathcal{H})\big), \quad z \in \rho(|\boldsymbol{D_A}|^2) \cap \rho(|\boldsymbol{D_A^*}|^2),$$
$$[g_z(A_+) - g_z(A_-)] \in \mathcal{B}_1(\mathcal{H}), \quad z \in \rho\big(A_+^2\big) \cap \rho\big(A_-^2\big),$$

and the following principal trace formula holds for all $z \in \mathbb{C}\backslash[0,\infty)$*,*

$$\operatorname{tr}_{L^2(\mathbb{R};\mathcal{H})}\Big(\big(|\boldsymbol{D_A^*}|^2 - z\big)^{-1} - \big(|\boldsymbol{D_A}|^2 - z\big)^{-1}\Big) = \frac{1}{2z}\operatorname{tr}_{\mathcal{H}}\big(g_z(A_+) - g_z(A_-)\big). \tag{3.4}$$

Remark 3.9.

(i) Pushnitski [54] was the first to investigate, under the more restrictive assumption that the operators $B(t)$ are *trace class*, a trace formula of this kind. In our more general setting of relative trace class perturbations, this formula is obtained in [30] by an approximation technique on both sides of the equation and a non-trivial DOI technique.

(ii) Employing basic notions in scattering theory and the Jost–Pais-type reduction of Fredholm determinant, a recent paper [23] provides a new proof of the principle trace formula in the case of trace class perturbations.

(iii) If $\mathcal{H} = \mathbb{C}$, the principal trace formula yields (3.1) for the example considered by D. Bolle *et al.* for $\phi_\pm = \pm 1$. $\diamond$

3.3. Pushnitski's formula relating two SSFs

Having at hand the principal trace formula, we now aim at correlating the underlying SSFs, $\xi(\,\cdot\,; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2)$ and $\xi(\,\cdot\,; A_+, A_-)$.

First, we need to properly introduce the SSF $\xi\big(\,\cdot\,; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big)$ associated with the pair of positive operators $|\boldsymbol{D}_{\boldsymbol{A}}^*|^2$ and $|\boldsymbol{D}_{\boldsymbol{A}}|^2$. By Theorem 3.8 we have

$$\Big[\big(|\boldsymbol{D}_{\boldsymbol{A}}^*|^2 - z\big)^{-1} - \big(|\boldsymbol{D}_{\boldsymbol{A}}|^2 - z\big)^{-1}\Big] \in \mathcal{B}_1\big(L^2(\mathbb{R}; \mathcal{H})\big),$$

and therefore, one can uniquely introduce $\xi\big(\,\cdot\,; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big)$ by requiring that

$$\xi\big(\lambda; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big) = 0, \quad \lambda < 0,$$

and then obtains

$$\operatorname{tr}_{L^2(\mathbb{R};\mathcal{H})}\Big(\big(|\boldsymbol{D}_{\boldsymbol{A}}^*|^2 - z\big)^{-1} - \big(|\boldsymbol{D}_{\boldsymbol{A}}|^2 - z\big)^{-1}\Big) = -\int_{[0,\infty)} \frac{\xi\big(\lambda; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big)\, d\lambda}{(\lambda - z)^2},$$

for all $z \in \mathbb{C}\backslash[0,\infty)$ (see Section 2.6).

We shall introduce the spectral shift function associated with the pair (A_+, A_-) via the invariance principle (see Section 2.6). By Theorem 3.8, $[g_{-1}(A_+) - g_{-1}(A_-)] \in \mathcal{B}_1(\mathcal{H})$ and so one can define the SSF $\xi(\,\cdot\,; A_+, A_-)$ for the pair (A_+, A_-) by setting

$$\xi(\nu; A_+, A_-) := \xi(g_{-1}(\nu); g_{-1}(A_+), g_{-1}(A_-)), \quad \nu \in \mathbb{R},$$

where $\xi(\,\cdot\,; g_{-1}(A_+), g_{-1}(A_-))$ is the spectral shift function associated with the pair $(g_{-1}(A_+), g_{-1}(A_-))$ uniquely determined by the requirement

$$\xi(\,\cdot\,; g_{-1}(A_+), g_{-1}(A_-)) \in L^1(\mathbb{R}; d\omega).$$

Therefore, by the Lifshitz–Krein trace formula (2.7),

$$\operatorname{tr}_{\mathcal{H}}\big(g_z(A_+) - g_z(A_-)\big) = -z \int_{\mathbb{R}} \frac{\xi(\nu; A_+, A_-)\, d\nu}{(\nu^2 - z)^{3/2}}, \quad z \in \mathbb{C}\backslash[0,\infty).$$

By the principal trace formula one obtains the equality

$$\begin{aligned}
&\int_{[0,\infty)} \frac{\xi\big(\lambda; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big)\, d\lambda}{(\lambda - z)^{-2}} \\
&\quad = -\operatorname{tr}_{L^2(\mathbb{R};\mathcal{H})}\Big(\big(|\boldsymbol{D}_{\boldsymbol{A}}^*|^2 - z\,\boldsymbol{I}\big)^{-1} - \big(|\boldsymbol{D}_{\boldsymbol{A}}|^2 - z\,\boldsymbol{I}\big)^{-1}\Big) \\
&\quad = -\frac{1}{2z} \operatorname{tr}_{\mathcal{H}}\big(g_z(A_+) - g_z(A_-)\big) \\
&\quad = \frac{1}{2} \int_{\mathbb{R}} \frac{\xi(\nu; A_+, A_-)\, d\nu}{(\nu^2 - z)^{3/2}}, \quad z \in \mathbb{C}\backslash[0,\infty),
\end{aligned}$$

or, equivalently,

$$\int_{[0,\infty)} \xi\big(\lambda; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big)\bigg(\frac{d}{dz}(\lambda - z)^{-1}\bigg) d\lambda$$
$$= \int_{\mathbb{R}} \xi(\nu; A_+, A_-)\bigg(\frac{d}{dz}(\nu^2 - z)^{-1/2}\bigg) d\nu.$$

Integrating the preceding equality with respect to z from a fixed point $z_0 \in (-\infty, 0)$ to $z \in \mathbb{C}\backslash\mathbb{R}$, along a straight line connecting z_0 and z, yields

$$\int_{[0,\infty)} \xi\big(\lambda; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big)\bigg(\frac{1}{\lambda - z} - \frac{1}{\lambda - z_0}\bigg) d\lambda$$
$$= \int_{\mathbb{R}} \xi(\nu; A_+, A_-)\big[(\nu^2 - z)^{-1/2} - (\nu^2 - z_0)^{-1/2}\big]\, d\nu, \quad z \in \mathbb{C}\backslash[0,\infty).$$

Applying the Stieltjes inversion formula then permits one to express the SSF function $\xi\big(\,\cdot\,; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big)$ in terms of $\xi(\,\cdot\,; A_+, A_-)$ as follows,

$$\xi\big(\lambda; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big) = \lim_{\varepsilon\downarrow 0} \frac{1}{\pi} \int_{[0,\infty)} \xi\big(\lambda'; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big) \operatorname{Im}\big(((\lambda' - \lambda) - i\varepsilon)^{-1}\big) d\lambda'$$
$$= \lim_{\varepsilon\downarrow 0} \frac{1}{\pi} \int_{\mathbb{R}} \xi(\nu; A_+, A_-) \operatorname{Im}\big((\nu^2 - \lambda - i\varepsilon)^{-1/2}\big) d\nu$$
$$= \frac{1}{\pi} \int_{-\lambda^{1/2}}^{\lambda^{1/2}} \frac{\xi(\nu; A_+, A_-)\, d\nu}{(\lambda - \nu^2)^{1/2}} \quad \text{for a.e. } \lambda > 0.$$

In the last equality here one should be careful with various estimates in order to apply Lebesgue's dominated convergence theorem. We omit further details and refer to [30].

Putting all of this together we have the following remarkable formula, which expresses the SSF, $\xi\big(\,\cdot\,; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big)$, in terms of the SSF $\xi(\,\cdot\,;; A_+, A_-)$. It is this formula that allows us to express (Fredholm/Witten) index of the operator $\boldsymbol{D}_{\boldsymbol{A}}$ in terms of the spectral shift function $\xi(\,\cdot\,; A_+, A_-)$. Note, that this formula can be viewed as an Abel-type transform.

Theorem 3.10 (Pushnitski's formula). *Assume Hypothesis* 3.5 *and define the spectral shift functions* $\xi\big(\,\cdot\,; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big)$ *and* $\xi(\,\cdot\,\,; A_+, A_-)$ *as above. Then, for a.e.* $\lambda > 0$,

$$\xi\big(\lambda; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big) = \frac{1}{\pi} \int_{-\lambda^{1/2}}^{\lambda^{1/2}} \frac{\xi(\nu; A_+, A_-)\, d\nu}{(\lambda - \nu^2)^{1/2}},$$

with a convergent Lebesgue integral on the right-hand side.

A formula of this kind was originally obtained for trace class perturbations $B(t)$ by Pushnitski [54] and in the generality presented above in [30].

3.4. The Fredholm case

In order to study the Witten index of the operator $\boldsymbol{D_A}$ we first need to understand under which additional assumptions this operator is Fredholm, which is of course the simpler case. The following result yields necessary and sufficient conditions for the latter.

Theorem 3.11 ([24, Theorem 2.6]). *Assume Hypothesis* 3.5. *Then the operator* $\boldsymbol{D_A}$ *is Fredholm if and only if* $0 \in \rho(A_+) \cap \rho(A_-)$ *(i.e.,* $A_\pm$ *are both boundedly invertible).*

In fact, this theorem yields a complete description of the essential spectrum of $\boldsymbol{D_A}$. Here we define the essential spectrum of a densely defined, closed, linear operator T in a complex, separable Hilbert space $\mathcal{H}$ as

$$\sigma_{\rm ess}(T) = \{\lambda \in \mathbb{C} \,|\, (T - \lambda I_{\mathcal{H}}) \text{ is not Fredholm}\}$$

(but caution the reader that several inequivalent, yet meaningful, definitions of essential spectra for non-self-adjoint operators exist, see, e.g., [26, Ch. IX]).

Corollary 3.12. [24, Corollary 2.8] *Assume Hypothesis* 3.5. *Then,*

$$\sigma_{\rm ess}(\boldsymbol{D_A}) = (\sigma(A_+) + i\,\mathbb{R}) \cup (\sigma(A_-) + i\,\mathbb{R}).$$

By Theorem 3.11, when the operator $\boldsymbol{D_A}$ is Fredholm, we have that $0 \in \rho(A_+) \cap \rho(A_-)$. Thus, by Corollary 3.12, $|\boldsymbol{D_A}|^2$ and $|\boldsymbol{D_A^*}|^2$ have a gap in their essential spectrum near zero, that is, there exists an $a > 0$ such that

$$\sigma_{\rm ess}\big(|\boldsymbol{D_A}|^2\big) = \sigma_{\rm ess}\big(|\boldsymbol{D_A^*}|^2\big) \subset [a, \infty).$$

This means that, on the interval $[0, a)$, the operators $|\boldsymbol{D_A}|^2$ and $|\boldsymbol{D_A^*}|^2$ have discrete spectra. Hence, using properties of the spectral shift function for discrete spectra (see property (iii) in Subsection 2.3) one infers that

$$\xi\big(\lambda; |\boldsymbol{D_A^*}|^2, |\boldsymbol{D_A}|^2\big) = \xi(0_+; |\boldsymbol{D_A^*}|^2, |\boldsymbol{D_A}|^2), \quad \lambda \in (0, \lambda_0),$$

for $\lambda_0 < \inf(\sigma_{\rm ess}(|\boldsymbol{D_A}|^2)) = \inf(\sigma_{\rm ess}(|\boldsymbol{D_A^*}|^2))$.

On the other hand, since $0 \in \rho(A_+) \cap \rho(A_-)$, there exists a constant $c \in \mathbb{R}$ such that $\xi(\,\cdot\,; A_+, A_-) = c$ a.e. on the interval $(-\nu_0, \nu_0)$ for $0 < \nu_0$ sufficiently small (see property (i) in Subsection 2.3). Hence, the value $\xi(0; A_+, A_-)$ is well defined and

$$\xi(\nu; A_+, A_-) = \xi(0; A_+, A_-), \quad \nu \in (-\nu_0, \nu_0),$$

in particular, $\lim_{\nu \to 0} \xi(\nu; A_+, A_-) = \xi(0; A_+, A_-)$.

Thus, taking $\lambda \downarrow 0$ in Pushnitski's formula one infers

$$\begin{aligned} \xi(0_+; |\boldsymbol{D_A^*}|^2, |\boldsymbol{D_A}|^2) &= \lim_{\lambda \downarrow 0} \xi(\lambda; |\boldsymbol{D_A^*}|^2, |\boldsymbol{D_A}|^2) \\ &= \lim_{\lambda \downarrow 0+} \frac{1}{\pi} \int_{-\lambda^{1/2}}^{\lambda^{1/2}} \frac{\xi(\nu; A_+, A_-)\, d\nu}{(\lambda - \nu^2)^{1/2}} = \lim_{\nu \to 0} \xi(\nu; A_+, A_-) = \xi(0; A_+, A_-) \end{aligned}$$

since $\pi^{-1} \int_{-\lambda^{1/2}}^{\lambda^{1/2}} d\nu\, (\lambda - \nu^2)^{-1/2} = 1$ for all $\lambda > 0$.

Thus, we obtain the following result linking the Fredholm index for $\boldsymbol{D_A}$ and the value of the SSF $\xi(\,\cdot\,; A_+, A_-)$ at zero.

Theorem 3.13 ([30]). *Assume Hypothesis* 3.5 *and introduce the SSFs* $\xi(\,\cdot\,; A_+, A_-)$ *and* $\xi\big(\,\cdot\,; |\boldsymbol{D_A^*}|^2, |\boldsymbol{D_A}|^2\big)$ *as above. Moreover, suppose that* $0 \in \rho(A_+) \cap \rho(A_-)$*. Then* $\boldsymbol{D_A}$ *is a Fredholm operator in* $L^2(\mathbb{R}; \mathcal{H})$ *and*

$$W_r(\boldsymbol{D_A}) = \operatorname{ind}(\boldsymbol{D_A}) = \xi\big(0_+; |\boldsymbol{D_A^*}|^2, |\boldsymbol{D_A}|^2\big) = \xi(0; A_+, A_-). \tag{3.5}$$

We emphasize that the assumption $0 \in \rho(A_+) \cap \rho(A_-)$ is crucial in the Fredholm index formula (3.5) of the operator $\boldsymbol{D_A}$. This assumption allows us to *define* the value of SSF $\xi(\,\cdot\,; A_+, A_-)$ at zero. Generally speaking, the SSF $\xi(\,\cdot\,; A_+, A_-)$ is defined as an element in $L^1\big(\mathbb{R}; (|\nu| + 1)^{-3}\big)$ (the space of classes of functions), so it does not make sense to speak of its value at a fixed point.

3.5. Connection to spectral flow

The relationship between spectral flow and the Fredholm index was first raised in the original articles of Atiyah–Patodi–Singer [7]. A definitive treatment of the question for certain families of self-adjoint unbounded operators with compact resolvent was provided in [55], essentially, using the model operator formalism that we described above. For partial differential operators on noncompact manifolds it is typically the case that they possess some essential spectrum so that [55] is not applicable. This motivated the investigation in [54] and [30]. The first of these papers introduces new methods and ideas, relating the index/spectral flow connection to scattering theory and the spectral shift function. However the conditions imposed in [54] are too restrictive to allow a wide class of examples. New tools were introduced in [30] as is explained above. A more detailed history of these matters may also be found in [23] which also contains results on an index theory for certain non-Fredholm operators using the model operator formalism above.

One of the principle aims of [30] was to extend the results in [55] (albeit subject to a relative trace class perturbation condition), in a fashion permitting essential spectra. This has motivated our interest in the problem of applying these new methods to Dirac-type operators on non-compact manifolds. There is a difficulty, however, in that the relative trace class perturbation assumption is not satisfied in this context (even in the one-dimensional case). In the last section of this review we will address this difficulty via a class of examples.

Spectral flow is usually discussed in terms of measuring the net number of eigenvalues of a one parameter family of Fredholm operators that change sign as one moves along the path. In fact we need a more precise definition and use the one due to Phillips [51].

Consider a norm continuous path F_t, $t \in [0; 1]$, of bounded self-adjoint Fredholm operators joining F_1 and F_0. For each t, we let P_t be the spectral projection of F_t corresponding to the non-negative reals. Then we can write $F_t = (2P_t - 1)|F_t|$. Phillips showed that if one subdivides the path into small intervals $[t_j, t_{j+1}]$ such that P_{t_j} and $P_{t_{j+1}}$ are "close" in the Calkin algebra, then they form a Fredholm pair (i.e., $P_{t_j}P_{t_{j+1}}$ is a Fredholm operator from $\operatorname{ran}(P_{t_{j+1}})$ to $\operatorname{ran}(P_{t_j})$) and the spectral flow along $\{F_t\}_{t\in[0,1]}$ is defined by

$$\sum\nolimits_j \operatorname{ind}(P_{t_j}P_{t_{j+1}} : \operatorname{ran}(P_{t_{j+1}}) \to \operatorname{ran}(P_{t_j})).$$

We will now state the main result of [30] on the connection between the spectral flow along the path $\{A(t)\}_{t\in\mathbb{R}}$ with the spectral shift functions and the Fredholm index of the model operator $\boldsymbol{D_A}$ introduced previously. However, first we need some preparatory observations.

First, we note that spectral flow along the path of unbounded operators $\{A(t)\}_{t\in\mathbb{R}}$ is defined in terms of the flow along the bounded transforms $\big\{F_t = A(t)(I+A(t)^2)^{-1/2}\big\}_{t\in\mathbb{R}}$ using Phillips' definition above. Next, we remark that the fact that the spectral shift function is relevant to the discussion of spectral flow was first noticed by Müller [48] and explained in a systematic fashion in 2007 in [9]. There it was shown that, under very general conditions guaranteeing that both are well defined, the spectral shift function and spectral flow are the same notion. The main technical tool exploited there is the theory of double operator integrals.

The new ingredient in [30] is a formula, which connects the spectral flow with both the spectral shift function and the Fredholm index. This formula applies independently of whether the operators in the path have non-trivial essential spectrum or not. More precisely, the spectral flow along the family of Fredholm operators $\{A(t)\}_{t\in\mathbb{R}}$ coincides with the value of the Fredholm index of the operator $\boldsymbol{D_A}$ and the value of the SSF, $\xi(\,\cdot\,; A_+, A_-)$, computed at zero.

Theorem 3.14 ([30]). *Assume Hypothesis* 3.5 *and suppose that* $0 \in \rho(A_+) \cap \rho(A_-)$. *Then* $\big(E_{A_+}((-\infty,0)), E_{A_-}((-\infty,0))\big)$ *form a Fredholm pair and the following equalities hold:*

$$\begin{aligned}\operatorname{SpFlow}(\{A(t)\}_{t=-\infty}^{\infty}) &= \operatorname{ind}(E_{A_-}(-\infty,0), E_{A_+}(-\infty,0))\\ &= \operatorname{tr}_{\mathcal{H}}(E_{A_-}(-\infty,0) - E_{A_+}(-\infty,0))\\ &= \xi(0; A_+, A_-) = \xi(0_+; \boldsymbol{H}_2, \boldsymbol{H}_1) = \operatorname{ind}(\boldsymbol{D_A}).\end{aligned}$$

4. Witten index: new results

In the preceding section we discussed the notion of the Witten index and its connection with the Fredholm index as well as the spectral shift function. As we already know from Theorem 3.11, the operator $\boldsymbol{D_A}$ is Fredholm if and only if $0 \in \rho(A_+) \cap \rho(A_-)$, that is, the operators $A_\pm$ are both boundedly invertible. Moreover, if $0 \in \rho(A_+) \cap \rho(A_-)$, then the Fredholm index can be computed as

$$\operatorname{ind}(\boldsymbol{D_A}) = \xi(0; A_+, A_-).$$

Here, the assumption $0 \in \rho(A_+) \cap \rho(A_-)$ is crucial, since in this case, there exists $0 < \nu \in \mathbb{R}$, such that $\xi(\,\cdot\,; A_+, A_-)$ is constant on the interval $(-\nu, \nu)$ so that one can speak about the value of the SSF, $\xi(\,\cdot\,; A_+, A_-)$, at zero. An important question then is to study an extension of index theory for the operator

$\boldsymbol{D}_{\boldsymbol{A}}$, when the latter ceases to be Fredholm. In this case $0 \in \sigma(A_+)$, or $0 \in \sigma(A_-)$ and therefore, the SSF $\xi(\,\cdot\,; A_+, A_-)$ *is not constant*, in general, on any interval $(-\nu, \nu), \nu > 0$.

An approach to computing the Witten indices $W_r(\boldsymbol{D}_{\boldsymbol{A}})$ (resp., $W_s(\boldsymbol{D}_{\boldsymbol{A}})$) suggested in [24] relies on the usage of right and left Lebesgue points of spectral shift functions. We start by briefly recalling this notion.

Definition 4.1. Let f be a locally integrable function on $\mathbb{R}$ and $h > 0$.

(i) The point $x \in \mathbb{R}$ is called a **right Lebesgue point** of f if there exists an $\alpha_+ \in \mathbb{C}$ such that
$$\lim_{h \downarrow 0} \frac{1}{h} \int_x^{x+h} dy\, |f(y) - \alpha_+| = 0.$$
We write $\alpha_+ = f_L(x_+)$.

(ii) The point $x \in \mathbb{R}$ is called a **left Lebesgue point** of f if there exists an $\alpha_- \in \mathbb{C}$ such that
$$\lim_{h \downarrow 0} \frac{1}{h} \int_{x-h}^{x} dy\, |f(y) - \alpha_-| = 0.$$
We write $\alpha_- = f_L(x_-)$.

(iii) The point $x \in \mathbb{R}$ is called a **Lebesgue point** of f if there exist $\alpha \in \mathbb{C}$ such that
$$\lim_{h \downarrow 0} \frac{1}{2h} \int_{x-h}^{x+h} dy\, |f(y) - \alpha| = 0.$$
We write $\alpha = f_L(x)$. That is, $x \in \mathbb{R}$ is a Lebesgue point of f if and only if it is a left and a right Lebesgue point and $\alpha_+ = \alpha_- = \alpha$.

We note that this definition of a Lebesgue point of f is not universally adopted. For instance, [34, p. 278] define x_0 to be a Lebesgue point of f if
$$\lim_{h \downarrow 0} \frac{1}{h} \int_0^h dy\, |f(x + y) + f(x_0 - y) - 2f(x)| = 0. \tag{4.1}$$

The elementary example
$$f(x; \beta) = \begin{cases} 0, & x < 0, \\ \beta, & x = 0, \\ 1, & x > 0, \end{cases} \quad \beta \in \mathbb{C},$$
shows that $f_L(0_+; \beta) = 1$ and $f_L(0_-; \beta) = 0$, that is, $x_0 = 0$ is a right and a left Lebesgue point of $f(\,\cdot\,; \beta)$ in the sense of Definitions 4.1, whereas there exists no $\beta \in \mathbb{C}$ such that $f(\,\cdot\,; \beta)$ satisfies (4.1) for $x_0 = 0$.

Everywhere below we use the terms left and right Lebesgue point of a function in the sense of Definition 4.1.

4.1. Connection between Lebesgue points of the SSFs, $\xi(\,\cdot\,; A_+, A_-)$ and $\xi\big(\,\cdot\,; |D_A^*|^2, |D_A|^2\big)$

As in the Fredholm case, the main ingredient in computing the Witten index is Pushnitski's formula (see Theorem 3.10):

$$\xi\big(\lambda; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big) = \frac{1}{\pi}\int_{-\lambda^{1/2}}^{\lambda^{1/2}} \frac{\xi(\nu; A_+, A_-)\,d\nu}{(\lambda-\nu^2)^{1/2}}.$$

We can rewrite this formula as follows:

$$\xi\big(\lambda; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big) = \frac{1}{\pi}\int_0^{\lambda^{1/2}} \frac{d\nu\,[\xi(\nu; A_+, A_-) + \xi(-\nu; A_+, A_-)]}{(\lambda-\nu^2)^{1/2}}, \quad \lambda > 0,$$

and consider the operator S, defined by setting

$$S : \begin{cases} L^1_{\text{loc}}(\mathbb{R}; d\nu) \to L^1_{\text{loc}}((0,\infty); d\lambda), \\ f \mapsto \frac{1}{\pi}\int_0^{\lambda^{1/2}} d\nu\,(\lambda-\nu^2)^{-1/2} f(\nu), \quad \lambda > 0, \end{cases} \tag{4.2}$$

We then have the following result for the operator S:

Lemma 4.2 ([24, Lemma 4.1]). *If* 0 *is a right Lebesgue point for* $f \in L^1_{\text{loc}}(\mathbb{R}; d\nu)$*, then it is also a right Lebesgue point for* Sf *and* $(Sf)_L(0_+) = \frac{1}{2} f_L(0_+)$*.*

Hence, assuming that 0 is a right and a left Lebesgue point of $\xi(\cdot; A_+, A_-)$, an application of this lemma to the particular function

$$f(\nu) = \xi(\nu; A_+, A_-) + \xi(-\nu; A_+, A_-),$$

$\nu > 0$, yields that 0 is a right Lebesgue point of $\xi\big(\,\cdot\,; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big)$ and

$$\xi_L\big(0_+; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big) \overset{\text{Lemma 4.2}}{=} [\xi_L(0_+; A_+, A_-) + \xi_L(0_-; A_+, A_-)]/2. \tag{4.3}$$

Thus, in the case, when $0 \in \sigma(A_+)$ (or $\sigma(A_-)$), we can still correlate the values at zero of the functions $\xi(\cdot; A_+, A_-)$ and $\xi\big(\,\cdot\,; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big)$ (in the Lebesgue point sense).

4.2. Computing the Witten index of the operator D_A

As a consequence of the principal trace formula, Theorem 3.8, and the Lifshitz–Krein trace formula, the following equality holds,

$$z\,\mathrm{tr}_{L^2(\mathbb{R};\mathcal{H})}\Big(\big(|\boldsymbol{D}_{\boldsymbol{A}}^*|^2 - z\,\boldsymbol{I}\big)^{-1} - \big(|\boldsymbol{D}_{\boldsymbol{A}}|^2 - z\,\boldsymbol{I}\big)^{-1}\Big) = -\frac{z}{2}\int_{\mathbb{R}} \frac{\xi(\nu; A_+, A_-)\,d\nu}{(\nu^2 - z)^{3/2}}, \tag{4.4}$$

for all $z \in \mathbb{C}\backslash[0,\infty)$. Recalling that the resolvent regularized Witten index $W_r(\boldsymbol{D}_{\boldsymbol{A}})$ is the limit of the LHS as $z \to 0$, $z < 0$, we see that this index can be computed by taking the limit of the RHS as $z \to 0$, $z < 0$. To this end, we consider the operator $\mathbf{T}$, defined by setting

$$\mathbf{T} : \begin{cases} L^1\big(\mathbb{R}; (1+\nu^2)^{-3/2} d\nu\big) \to \mathrm{Hol}(\mathbb{C}\backslash[0,\infty)) \\ f \mapsto -z\int_{\mathbb{R}} d\nu\,(\nu^2 - z)^{-3/2} f(\nu), \quad z \in \mathbb{C}\backslash[0,\infty), \end{cases}$$

where $\mathrm{Hol}(\mathbb{C}\backslash[0,\infty))$ denotes the set of all holomorphic functions on $\mathbb{C}\backslash[0,\infty)$.

Lemma 4.3 ([24]). *If* 0 *is a left and a right Lebesgue point for* $f \in L^1\big(\mathbb{R};(1+\nu^2)^{-3/2}d\nu\big)$, *then*

$$\lim_{z\uparrow 0}(\mathbf{T}f)(z) = f_L(0_+) + f_L(0_-). \tag{4.5}$$

Thus, applying this lemma to the function $\xi(\,\cdot\,;A_+,A_-)$ on the right-hand side of (4.4), we arrive at the equality

$$\begin{aligned} W_r(\boldsymbol{D_A}) &= \lim_{z\uparrow 0} z\,\mathrm{tr}_{L^2(\mathbb{R};\mathcal{H})}\Big(\big(|\boldsymbol{D_A^*}|^2 - z\,\boldsymbol{I}\big)^{-1} - \big(|\boldsymbol{D_A}|^2 - z\,\boldsymbol{I}\big)^{-1}\Big) \\ &= \lim_{z\uparrow 0} -\frac{z}{2}\int_{\mathbb{R}} \frac{\xi(\nu;A_+,A_-)\,d\nu}{(\nu^2-z)^{3/2}} \\ &= \frac{1}{2}\lim_{z\uparrow 0}(\mathbf{T}\xi(\,\cdot\,;A_+,A_-))(z) \overset{\text{Lemma 4.3}}{=} [\xi_L(0_+)+\xi_L(0_-)]/2. \end{aligned}$$

Now, we turn to computing the semigroup regularized Witten index $W_s(\boldsymbol{D_A})$. To this end, we have established the following

Theorem 4.4 ([24]). *If* 0 *is a right Lebesgue point of* $\xi\big(\,\cdot\,;|\boldsymbol{D_A^*}|^2,|\boldsymbol{D_A}|^2\big)$, *then*

$$\lim_{z\to\infty, z>0} \mathrm{tr}_{L^2(\mathbb{R};\mathcal{H})}\Big(e^{-z|\boldsymbol{D_A^*}|^2} - e^{-z|\boldsymbol{D_A}|^2}\Big) = \xi_L\big(0_+;|\boldsymbol{D_A^*}|^2,|\boldsymbol{D_A}|^2\big),$$

uniformly with respect to z.

Therefore, if 0 is a right and a left Lebesgue point of $\xi(\,\cdot\,;A_+,A_-)$, then combining this theorem with equality (4.3) we obtain

$$W_s(\boldsymbol{D_A}) = \xi_L\big(0_+;|\boldsymbol{D_A^*}|^2,|\boldsymbol{D_A}|^2\big) \overset{\text{Lemma 4.2}}{=} [\xi_L(0_+)+\xi_L(0_-)]/2.$$

Theorem 4.5 ([24, Theorem 4.3]). *Assume Hypothesis* 3.5 *and suppose that* 0 *is a right and a left Lebesgue point of* $\xi(\,\cdot\,;A_+,A_-)$. *Then* 0 *is a right Lebesgue point of* $\xi\big(\,\cdot\,;|\boldsymbol{D_A^*}|^2,|\boldsymbol{D_A}|^2\big)$ *and*

$$\xi_L\big(0_+;|\boldsymbol{D_A^*}|^2,|\boldsymbol{D_A}|^2\big) = [\xi_L(0_+;A_+,A_-)+\xi_L(0_-;A_+,A_-)]/2.$$

and

$$W_r(\boldsymbol{D_A}) = [\xi_L(0_+;A_+,A_-)+\xi_L(0_-;A_+,A_-)]/2 = W_s(\boldsymbol{D_A}).$$

We emphasize that Theorem 4.5 contains Theorem 3.13 as a particular case. Indeed, suppose that the operator $\boldsymbol{D_A}$ is Fredholm, that is, the asymptotes $A_\pm$ are boundedly invertible. In this case, 0 is a right and a left Lebesgue point of $\xi(\,\cdot\,;A_+,A_-)$ and $[\xi_L(0_+;A_+,A_-)+\xi_L(0_-;A_+,A_-)]/2 = \xi(0;A_+,A_-)$.

In the next subsection we discuss the case when 0 may belong to the spectra of the operators A_+ and A_-. As we already noted the Witten index, in general, can be any prescribed real number. Next we demonstrate that this also applies to the special case of the Witten index of the model operator $\boldsymbol{D_A}$.

A simple concrete example is the following: Consider $A_\pm \in \mathcal{B}(\mathcal{H})$ with $[A_+ - A_-] \in \mathcal{B}_1(\mathcal{H})$, and introduce the family

$$A(t) = A_- + e^t(e^t+1)^{-1}[A_+ - A_-], \quad t\in\mathbb{R},$$

which satisfies Hypothesis 3.5. Moreover, since *any* integrable function $\xi \in L^1(\mathbb{R};dt)$ of compact support arises as the spectral shift function for a pair of bounded, self-adjoint operators (A_+, A_-) in $\mathcal{H}$ with $[A_+ - A_-] \in \mathcal{B}_1(\mathcal{H})$, Theorem 4.5 implies that

$$\begin{aligned} W_r(\boldsymbol{D_A}) = W_s(\boldsymbol{D_A}) &= \xi_L(0; A_+, A_-) \\ &= \text{ any prescribed real number.} \end{aligned}$$

4.3. The spectra of $A_\pm$ and Lebesgue points of $\xi(\,\cdot\,; A_+, A_-)$

We start with the simpler case where $A_\pm$ have discrete spectrum in an open neighbourhood of 0. That is we assume, that for some $\nu > 0$, the interval $(-\nu, \nu)$ contains only eigenvalues of $A_\pm$ of *finite multiplicities*, which are *isolated points* in $\sigma(A_\pm)$. The following remark easily follows from properties of SSF (see Subsection 2.3, property (iii)).

Remark 4.6. If $A_\pm$ have discrete spectra in an open neighborhood of 0, then the SSF $\xi(\,\cdot\,; A_+, A_-)$ has a right and left limit at any point of this open neighborhood and, in particular, any point in that open neighborhood is a right and a left Lebesgue point of $\xi(\,\cdot\,; A_+, A_-)$. ◇

On the contrary, in the presence of purely absolutely continuous spectrum of $A_\pm$ in a neighborhood of 0, the situation is more complicated.

Proposition 4.7 ([24, Proposition 4.6]). *There exist pairs of bounded self-adjoint operators (A_+, A_-) in $\mathcal{H}$ such that $(A_+ - A_-)$ is of rank-one, and $A_\pm$ both have purely absolutely continuous spectrum in a fixed neighborhood $(-\varepsilon_0, \varepsilon_0)$, for some $\varepsilon_0 > 0$, yet $\xi(\,\cdot\,; A_+, A_-)$* may or may not have *a right and/or a left Lebesgue point at* 0.

4.4. The Witten index of $\boldsymbol{D_A}$ in the Special Case $\dim(\mathcal{H}) < \infty$

We briefly treat the special finite-dimensional case, $\dim(\mathcal{H}) < \infty$, and explicitly compute the Witten index of $\boldsymbol{D_A}$ *irrespectively* of whether or not $\boldsymbol{D_A}$ is a Fredholm operator in $L^2(\mathbb{R}; \mathcal{H})$.

In this special case the Hypothesis 3.5 acquires a considerably simpler form. We just suppose that

$$A_- \in \mathcal{B}(\mathcal{H}) \;\text{ is a self-adjoint matrix in } \mathcal{H}, \tag{4.6}$$

and there exists a family of bounded self-adjoint matrices $\{A(t)\}_{t\in\mathbb{R}}$, locally absolutely continuous on $\mathbb{R}$, such that

$$\int_{\mathbb{R}} dt\, \big\|A'(t)\big\|_{\mathcal{B}(\mathcal{H})} < \infty. \tag{4.7}$$

In the following we denote by $\#_>(S)$ (respectively $\#_<(S)$) the number of strictly positive (respectively, strictly negative) eigenvalues of a self-adjoint matrix S in $\mathcal{H}$, counting multiplicity. Under these assumptions the formula for the Witten index of the operator $\boldsymbol{D_A}$ takes a particularly simple form. If should be pointed out that the result below yields (in a very special setting where $\dim(\mathcal{H}) = 1$) the result of Example 3.4.

Theorem 4.8 ([24, Theorem 5.2]). *Assume Hypotheses* (4.6) *and* (4.7)*. Then the SSF* $\xi(\,\cdot\,; A_+, A_-)$ *has a piecewise constant representative on* $\mathbb{R}$*, the right limit* $\xi\big(0_+; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big)$ *exists, and the SSF* $\xi\big(\,\cdot\,; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big)$ *has a continuous representative on* $(0,\infty)$*. Moreover, the resolvent and semigroup regularized Witten indices* $W_r(\boldsymbol{D}_{\boldsymbol{A}})$ *and* $W_s(\boldsymbol{D}_{\boldsymbol{A}})$ *exist, and*

$$\begin{aligned} W_r(\boldsymbol{D}_{\boldsymbol{A}}) = W_s(\boldsymbol{D}_{\boldsymbol{A}}) &= \xi\big(0_+; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D}_{\boldsymbol{A}}|^2\big) \\ &= [\xi(0_+; A_+, A_-) + \xi(0_-; A_+, A_-)]/2 \\ &= \frac{1}{2}[\#_>(A_+) - \#_>(A_-)] - \frac{1}{2}[\#_<(A_+) - \#_<(A_-)]. \end{aligned}$$

In particular, in the finite-dimensional context, the Witten indices are either integer, or half-integer-valued.

5. Further extensions

In this section we discuss an important example of operators A_+ and A_-, whose spectra are absolutely continuous and coincide with the whole real line and for which the results of previous sections are not applicable. The results of [54] and [30], [24] describe the Fredholm/Witten index theory for operators permitting essential spectra but the relatively trace class assumption rules out standard partial differential operators such as Dirac type operators. Thus, in order to incorporate this important class of examples, we need a more general framework.

To illustrate this fact, we consider the following example. Let A_- and $\{A(t)\}_{t\in\mathbb{R}}$ be given by

$$A_- = \frac{d}{idx}, \quad A(t) = A_- + \theta(t)M_f, \quad \operatorname{dom}(A_-) = \operatorname{dom}(A(t)) = W^{1,2}(\mathbb{R}), \quad t \in \mathbb{R},$$

that is, we consider the differentiation operator on $L^2(\mathbb{R}; dx)$ and its perturbation by multiplication operator M_f defined by a function $f \in L^\infty(\mathbb{R}; dx)$. Here θ is a function satisfying

$$\begin{gathered} 0 \leqslant \theta \in L^\infty(\mathbb{R}; dt), \;\; \theta' \in L^\infty(\mathbb{R}; dt) \cap L^1(\mathbb{R}; dt), \\ \lim_{t\to-\infty} \theta(t) = 0, \quad \lim_{t\to+\infty} \theta(t) = 1. \end{gathered}$$

Then the asymptotes $A_\pm$ of the family $\{A(t)\}_{t\in\mathbb{R}}$ as $t \to \pm\infty$ are given by A_- and

$$A_+ = A_- + M_f.$$

In other words, we have a one-dimensional Dirac operator and its perturbation by a bounded function. The well-known Cwikel estimates (see, e.g., [56, Ch. 4]) guarantee that for f decaying sufficiently rapidly at $\pm\infty$, the operator $(A_+ - A_-)(A_-^2 + 1)^{-s/2}$ is trace class for $s > 1$, but for no lesser value of s. Thus, even in one dimension, the relative trace class assumption is violated for the example above.

However, although the one-dimensional differential operator A_- and its perturbations do not satisfy the relative trace class assumption, we still can compute the Witten index $W_r(\boldsymbol{D_A})$. For this one-dimensional setting, under the identification of the Hilbert spaces $L^2(\mathbb{R}; dt; L^2(\mathbb{R}; dx))$ and $L^2(\mathbb{R}^2; dtdx)$, the operator $\boldsymbol{D_A}$, defined by (3.2), is given by

$$\boldsymbol{D_A} = \frac{\mathbf{d}}{\mathbf{dt}} + \boldsymbol{A},$$

with $\boldsymbol{A} = \frac{d}{idx} + M_\theta M_f$. That is, in this setting we work with the operator

$$\boldsymbol{D_A} = \frac{\partial}{\partial t} + \frac{\partial}{i\partial x} + M_\theta M_f.$$

Since the operator $\frac{d}{idx}$ has absolutely continuous spectrum, coinciding with the whole real line, the operator $\boldsymbol{D_A}$ possesses the following properties:

(i) Since $0 \in \sigma(A_-) = \mathbb{R}$, by Theorem 3.11 we have that the operator $\boldsymbol{D_A}$ is *not Fredholm.*

(ii) The essential spectrum of the operator $\boldsymbol{D_A}$ is the *whole complex plane* $\mathbb{C}$ (see Corollary 3.12).

It is interesting (and somewhat surprising) that for this particular example under some assumptions on the perturbation f (see Theorem 5.1 below) we still have the inclusions (cf. Theorem 3.8)

$$[g_z(A_+) - g_z(A_-)] \in \mathcal{B}_1(L^2(\mathbb{R})),$$
$$\Big(\big(|\boldsymbol{D}_{\boldsymbol{A}}^*|^2 - z\,\boldsymbol{I}\big)^{-1} - \big(|\boldsymbol{D_A}|^2 - z\,\boldsymbol{I}\big)^{-1}\Big) \in \mathcal{B}_1\big(L^2\big(\mathbb{R}^2\big)\big), \quad z \in \mathbb{C}\backslash[0,\infty),$$

where $g_z(x) = x(x^2 - z)^{-1/2}$, $x \in \mathbb{R}$. Moreover, using an approximation technique, we can prove the principal trace formula as in Theorem 3.8

$$\operatorname{tr}_{L^2(\mathbb{R}^2)}\Big(\big(|\boldsymbol{D}_{\boldsymbol{A}}^*|^2 - z\,\boldsymbol{I}\big)^{-1} - \big(|\boldsymbol{D_A}|^2 - z\,\boldsymbol{I}\big)^{-1}\Big) = \frac{1}{2z}\operatorname{tr}_{L^2(\mathbb{R})}(g_z(A_+) - g_z(A_-)),$$

for all $z \in \mathbb{C}\backslash[0,\infty)$.

The main application of this principal trace formula is an extension of Pushnitski's formula. Furthermore, employing some classical harmonic analysis we are able to compute the *actual value* of (a representative of) the spectral shift function for the pair A_+, A_-.

Theorem 5.1. *Let $f \in W^{1,1}(\mathbb{R}; dx) \cap C_b(\mathbb{R}; dx)$ and $f' \in L^\infty(\mathbb{R}; dx)$. Then for a.e. $\lambda > 0$ and a.e. $\nu \in \mathbb{R}$,*

$$\xi\big(\lambda; |\boldsymbol{D}_{\boldsymbol{A}}^*|^2, |\boldsymbol{D_A}|^2\big) = \xi(\nu; A_+, A_-) = \frac{1}{2\pi}\int_{\mathbb{R}} f(x)\,dx.$$

The fact that the SSF $\xi(\,\cdot\,; A_+, A_-)$ is a constant immediately implies that 0 is Lebesgue point of the function $\xi(\,\cdot\,; A_+, A_-)$.

Theorem 5.2 ([21]). *The Witten indices* $W_r(\boldsymbol{D_A})$ *and* $W_s(\boldsymbol{D_A})$ *of the operator* $\boldsymbol{D_A}$ *exist and equal*

$$W_r(\boldsymbol{D_A}) = W_s(\boldsymbol{D_A}) = \xi\big(0_+; |\boldsymbol{D_A^*}|^2, |\boldsymbol{D_A}|^2\big) = \xi(0; A_+, A_-) = \frac{1}{2\pi}\int_{\mathbb{R}} f(x)dx.$$

Remark 5.3. We note that the equality $\xi(\,\cdot\,; A_+, A_-) = \frac{1}{2\pi}\int_{\mathbb{R}} f(x)dx$ may also be proved via scattering theory and modified Fredholm determinants of 2nd order (cf. [21]). ◇

The results above can be also generalized to the following setting. Assume that A_- is an (unbounded) self-adjoint operator in a complex separable Hilbert space $\mathcal{H}$ and assume that the family of bounded operators $\{B(t)\}_{t\in\mathbb{R}}$ is a 2-relative trace class perturbation, that is, $B'(t)(|A_-|+1)^{-2} \in \mathcal{B}_1(\mathcal{H})$, $t \in \mathbb{R}$, and

$$\int_{\mathbb{R}} dt\, \big\|B'(t)(|A_-|+1)^{-2}\big\|_{\mathcal{B}_1(\mathcal{H})} < \infty.$$

Imposing some minor additional conditions on the family $\{B(t)\}_{t\in\mathbb{R}}$ one can prove the following result:

Theorem 5.4. *Suppose that* 0 *is a right and a left Lebesgue point of* $\xi(\,\cdot\,; A_+, A_-)$*, then* 0 *is also a right Lebesgue point of* $\xi\big(\,\cdot\,; |\boldsymbol{D_A^*}|^2, |\boldsymbol{D_A}|^2\big)$ *and* $W_r(\boldsymbol{D_A})$ *exists and equals*

$$W_r(\boldsymbol{D_A}) = \xi_L\big(0_+; |\boldsymbol{D_A^*}|^2, |\boldsymbol{D_A}|^2\big) = [\xi_L(0_+; A_+, A_-) + \xi_L(0_-; A_+, A_-)]/2.$$

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Stahl's Theorem (aka BMV Conjecture): Insights and Intuition on its Proof

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Abstract. The Bessis–Moussa–Villani conjecture states that the trace of $\exp(A - tB)$ is, as a function of the real variable t, the Laplace transform of a positive measure, where A and B are respectively a hermitian and positive semi-definite matrix. The long standing conjecture was recently proved by Stahl and streamlined by Eremenko. We report on a more concise yet self-contained version of the proof.

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1. Statement

In 1975, Bessis Moussa and Villani conjectured in [1] a way of rewriting the partition function of a broad class of statistical systems. The precise statement can be formulated as follows.

Theorem 1 (Stahl's Theorem). *Let A and B be two $n \times n$ Hermitian matrices, where B is positive semidefinite. Then the function*

$$f(t) := Tr\, e^{A-tB}, \quad t \geq 0 \tag{1}$$

can be represented as the Laplace transform of a non-negative measure μ. That is,

$$f(t) = \int_0^\infty e^{-ts} d\mu(s). \tag{2}$$

More than 30 years later, Stahl published a proof of this conjecture in [2]. A minimal version of the proof has meanwhile been published by Eremenko in [3]. Our aim is to reconcile the exactness of Stahl's version of the proof with the clarity of Eremenko's version.

Intuitive Case. To get a feeling of why the above theorem holds, let us investigate the case where A and B commute.

Since our matrices are simultaneously diagonalisable, we can w.l.o.g. assume that they are given in diagonal form and exponentiating them becomes trivial. We therefore have:

$$f(t) = Tr\, e^{A-tB} = \sum_{j=1}^{n} e^{a_j} e^{-tb_j}. \tag{3}$$

We next define the measure $\mu := \sum_{j=1}^{n} e^{a_j} \delta_{b_j}$, where a_j and b_j are the matrix elements of A and B, and δ_{b_j} is the Dirac measure on $\mathbb{R}$. By noting that for any function $g(s)$, $\int_0^\infty g(s) d\delta_{b_j} = g(b_j)$, one immediately sees that

$$\int_0^\infty e^{-ts} d\mu(s) = \sum_{j=1}^{n} e^{a_j} e^{-tb_j} = f(t); \tag{4}$$

showing that, in the case of commuting matrices, the BMV conjecture is realized with a discrete positive μ.

To simplify the analysis of the general case, we first prove the following

Assumption. W.l.o.g. B can be assumed to have distinct positive eigenvalues $b_n > \cdots > b_1 > 0$.

Proof. Let $B \geq 0$. We work in the diagonal basis of B. We define $B_\varepsilon := B + \varepsilon\, D$ with $D = diag(1, 2, \ldots, n)$. Assuming Theorem 1 holds for B_ε, we want to prove it also holds for B; that is, assuming μ_ε exists and is non-negative, we want to prove μ exists and is non-negative.

Since the following involves the inverse Laplace transform, it is convenient to write the objects as tempered distributions. Explicitly,

$$\begin{aligned} \mu_\varepsilon[\varphi] &:= \int_0^\infty \varphi(s) d\mu_\varepsilon(s), \\ f_\varepsilon[\varphi] &:= \int_0^\infty \varphi(s) f_\varepsilon(s) ds; \end{aligned} \tag{5}$$

for test functions $\varphi \in C_0^\infty(\mathcal{R}^+)$. We note that $\mu_\varepsilon \geq 0 \Leftrightarrow \mu_\varepsilon[\varphi] \geq 0, \forall \varphi \geq 0$. Denoting the Laplace transform by $\mathcal{L}$, we have:

$$\mathcal{L}(\mu_\varepsilon)[\varphi] := \mu_\varepsilon[\mathcal{L}(\varphi)] = f_\varepsilon[\varphi], \tag{6}$$

which using the Bromwich integral formula yields

$$\mu_\varepsilon[\varphi] = \mathcal{L}^{-1}(f_\varepsilon)[\varphi] = \frac{1}{2\pi i} \int_{x-i\infty}^{x+i\infty} f_\varepsilon(z) \left(\int_0^\infty e^{z(s)} \varphi(s) ds \right) dz. \tag{7}$$

Using the Dominated Convergence Theorem one shows that (see Appendix A of [4])

$$\lim_{\varepsilon \to 0} \mu_\varepsilon[\varphi] = \frac{1}{2\pi i} \int_{x-i\infty}^{x+i\infty} f(z) \left(\int_0^\infty e^{z(s)} \varphi(s) ds \right) dz \geq 0\ ,\ \forall \varphi \geq 0, \tag{8}$$

where the inequality comes from $\mu_\varepsilon[\varphi] \geq 0$, $\forall \varphi \geq 0$. So with

$$\mu[\varphi] := \frac{1}{2\pi i}\int_{x-i\infty}^{x+i\infty} f(z)\left(\int_0^\infty e^{z(s)}\varphi(s)ds\right)dz, \tag{9}$$

we have $f = \mathcal{L}(\mu)$ and $\mu \geq 0$. □

2. Eigenvalues of $A - tB$

We tackle the general case by looking at $\lambda_1(t), \ldots, \lambda_n(t)$; the eigenvalues of $A - tB$.

Theorem 2.

i) $\lambda_1, \ldots, \lambda_n$ *have no branch point over* $\mathbb{R}$.
ii) $\lambda_1, \ldots, \lambda_n$ *are analytic in a neighborhood of infinity and* $\forall j = 1, \ldots, n$

$$\lambda_j(t) = a_{jj} - tb_j + \mathcal{O}(\frac{1}{t})\ (t \to \infty). \tag{10}$$

Proof. We want to study

$$\begin{aligned} &\det\left(\lambda(t)\, id - (A - tB)\right) = 0 \text{ as } t \to \infty \\ \Leftrightarrow &\det\left(b(u)\, id - (B + uA)\right) = 0 \text{ as } u \to 0, \end{aligned} \tag{11}$$

with

$$u := -\frac{1}{t} \text{ and } b(u) := u \cdot \lambda\left(-\frac{1}{u}\right). \tag{12}$$

That is, we are interested in the form of $b(u)$, the slightly perturbed (isolated) eigenvalues of B. Fortunately, this finds an answer in most text books on Quantum Mechanics. See, e.g., Ch. 11.1 of [5] for an intuitive approach or Ch. XII of [6] for a rigorous one. In any case, one finds for $j = 1, \ldots, n$:

$$b_j(u) = b_j + ua_{jj} + \mathcal{O}(u^2)\ (u \to 0). \tag{13}$$

Analyticity and uniqueness of $b_j(u)$ near $u = 0$ is assured by Theorem XII.1 in [6] and since $B + uA$ is self adjoint $\forall u \in \mathbb{R}$, by Rellich's Theorem (Theorem XII.3 in [6]), $b_i(u)$ is analytic and single-valued in a neighborhood of u_0, $\forall u_0 \in \mathbb{R}$. Plugging definition 12 in equation 13 we therefore have for $j = 1, \ldots, n$ that

$$\lambda_j(t) = a_{jj} - tb_j + \mathcal{O}\left(\frac{1}{t}\right)(t \to \infty) \tag{14}$$

is analytic in a neighborhood of infinity and has no branch point over $\mathbb{R}$. □

3. Explicit form of μ

We now postulate an explicit form for μ.

Theorem 3. *The measure* $\mu := \omega + \sum_{j=i}^{n} e^{a_{jj}} \delta_{b_j}$ *satisfies*

$$f(t) = \int_0^\infty e^{-ts} d\mu(s), \tag{15}$$

for $f(t) = \operatorname{Tr} e^{A-tB}$ *and* $d\omega(s) := \omega(s)ds$*, where*

$$\omega(s) := \frac{1}{2\pi i} \sum_{j:\, b_j < s} \int_{\partial U} e^{\lambda_j(z)+sz} dz; \tag{16}$$

with U *a neighborhood of infinity such that* ∂U *is a positively oriented Jordan curve around zero.*

Before verifying Theorem 3, we prove the useful

Lemma 4. $\operatorname{supp}(\omega) \subset [b_1, b_n]$.

Proof. For $s \leq b_1$ the sum $\sum_{j:b_j<s}$ is void and hence trivially $\omega(s) = 0$. For $s > b_n$ we have:

$$2\pi i\, \omega(s) = \sum_{j=1}^{n} \int_{\partial U} e^{\lambda_j(z)+sz} dz = \int_{\partial U} \operatorname{Tr} e^{A-zB} e^{sz} dz, \tag{17}$$

where we used the spectral decomposition definition of e^{A-zB}, that is

$$e^{A-zB} := \sum_{\lambda} e^{\lambda} P_\lambda; \quad \lambda\text{: Eigenvalue of } A - zB. \tag{18}$$

Equivalently, see, e.g., [7], one can define e^{A-zB} through

$$e^{A-zB} := \frac{1}{2\pi} \int_\gamma \left(z'\, id - (A - zB)\right)^{-1} e^{z'} dz', \tag{19}$$

with γ enclosing the spectrum of $A - zB$, thereby ensuring $\left(z'\, id - (A - zB)\right)^{-1}$ to be well defined for $z' \in \gamma$ and in fact analytic as a function of z, since for any fixed $z' \in \gamma$ we have that

$$\frac{d}{dz} \left(z'\, id - (A - zB)\right)^{-1} = - \left(z'\, id - (A - zB)\right)^{-1} \left(\frac{d}{dz} \left(z'\, id - (A - zB)\right)\right) \left(z'\, id - (A - zB)\right)^{-1}. \tag{20}$$

With definition 19 we therefore see that $\operatorname{Tr} e^{A-zB}$ is analytic and hence by Cauchy's Theorem $\omega(s) = 0$. □

Proof of Theorem 3. We want to verify that $\mathcal{L}(\mu) = f$.

The first part of μ is the expression we found in the intuitive case of Section 1. Using Lemma 4 and noting that $\sum_{j:b_j<s} = \sum_{j=1}^{k}$ for $s \in (b_k, b_{k+1}]$, we find for the second one

$$\mathcal{L}(\omega)(t) = \int_{b_1}^{b_n} e^{-ts}\omega(s)ds = \sum_{k=1}^{n-1} I_k(t), \tag{21}$$

with

$$I_k = \frac{1}{2\pi i}\int_{b_k}^{b_{k+1}} \left(\sum_{j=1}^{k} \int_{\partial U} e^{\lambda_j(z)+s(z-t)}dz \right) ds. \tag{22}$$

Since according to Theorem 2 the λ_j's have no branch point over $\mathbb{R}$, by Cauchy's Theorem, we can, without altering the result of the integral, deform U to U_1, with U_1 as in Figure 1. Inverting the sums, i.e., $\sum_{k=1}^{n-1}\sum_{j=1}^{k} = \sum_{j=1}^{n-1}\sum_{k=j}^{n-1}$, and performing the s-integral, we then get

$$\sum_{k=1}^{n-1} I_k = \underbrace{\frac{1}{2\pi i}\sum_{j=1}^{n}\int_{\partial U_1} e^{\lambda_j(z)}\frac{e^{b_n(z-t)}}{z-t}dz}_{\diamondcircle} - \underbrace{\frac{1}{2\pi i}\sum_{j=1}^{n}\int_{\partial U_1} e^{\lambda_j(z)}\frac{e^{b_j(z-t)}}{z-t}dz}_{\circledast}. \tag{23}$$

Note that the n^{th} summand of $\diamondcircle$ and $\circledast$ cancel each other.

Since $f(z)\frac{e^{b_n(z-t)}}{z-t}$ is entire in $(U_1)^c$, we have by Cauchy's Theorem

$$\diamondcircle = \frac{1}{2\pi i}\int_{\partial U_1} f(z)\frac{e^{b_n(z-t)}}{z-t}dz = 0. \tag{24}$$

To evaluate $\circledast$ we first split the integration path:

$$\circledast = \sum_{j=1}^{n}\left[\underbrace{\frac{1}{2\pi i}\int_{\partial U_1 - C} e^{\lambda_j(z)}\frac{e^{b_j(z-t)}}{z-t}dz}_{①} + \underbrace{\frac{1}{2\pi i}\int_{C} e^{\lambda_j(z)}\frac{e^{b_j(z-t)}}{z-t}dz}_{②} \right], \tag{25}$$

with C a positively oriented curve with trace $\{z:\ |z| = R > t\}$ as depicted in Figure 1. Since $z = t$ is the only pole enclosed by $\partial U_1 - C$, using the residue theorem, $① = -e^{\lambda_j(t)}$. We then rewrite ② using Theorem 2 to express λ_j as

$$\lambda_j(z) = -b_j z + a_{jj} + r_j(z), \tag{26}$$

where r_j is analytic in U_1 and $r_j(\infty) = 0$. So

$$② = e^{a_{jj}-b_j t}\frac{1}{2\pi i}\int_C \frac{e^{r_j(z)}}{z-t}dz. \tag{27}$$

Performing the change of variable $z := 1/z$, the new variable integrates over

$$\frac{1}{C}: \text{negatively oriented curve with trace } \left\{z:\ |z| = \frac{1}{R}\right\}, \tag{28}$$

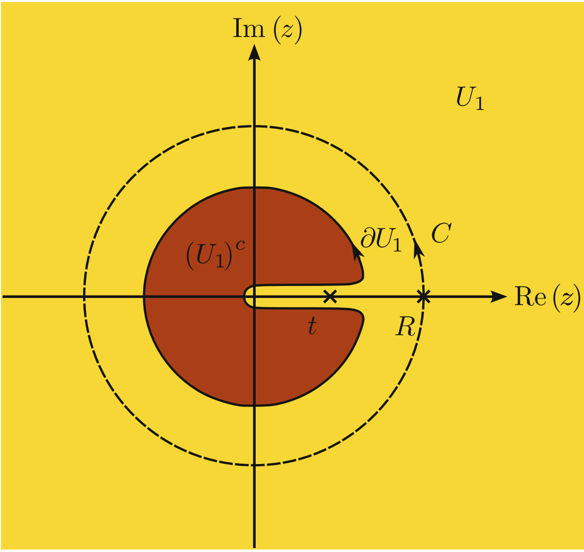

FIGURE 1. The choice of U_1, in yellow, is made such that $t \in U_1$. Such a choice is enabled by Theorem 2 i).

and we therefore get

$$\textcircled{2} = -e^{a_{jj}-b_j t} \frac{1}{2\pi i} \int_{\frac{1}{C}} \frac{e^{r_j(z^{-1})}}{z(1-tz)} dz = e^{a_{jj}-b_j t} e^{r_k(\infty)} = e^{a_{jj}-b_j t}; \tag{29}$$

since as $|z| = 1/R < 1/t$, the only pole of the integrand is at $z = 0$.

Gathering the results of ①, ②, ⊛ and ◈ we get

$$\mathcal{L}(\omega)(t) = -\circledast = -\sum_{j=1}^{n} e^{a_{jj}-b_j t} + \operatorname{Tr} e^{A-tB}, \tag{30}$$

which with the result of the intuitive case gives $\mathcal{L}(\mu)(t) = \operatorname{Tr} e^{A-tB}$. □

4. Domain of definition of $\boldsymbol{\lambda}$

We would now like to talk about λ, the solution of $det\,(\lambda(t)\,id - (A - tB)) = 0$, in a global fashion instead of viewing it as n different functions $\lambda_1, \ldots, \lambda_n$. A fruitful way to do so is to define its domain of definition, S, as a Riemann surface; for further reading see [8] or [9].

We choose the n sheets of S, S_j $(j = 1, \ldots, n)$, such that in the neighborhood of infinity where we already numbered the λ_j's (see Theorem 2) we have that

$$\lambda_j = \lambda \circ \pi_j^{-1}, \tag{31}$$

with $\pi : S \to \bar{\mathbb{C}}$ the canonical projection of S and π_j its restriction to S_j.

We further denote the lifting of the complex conjugate over S by ρ and note that since λ is of real type, $\rho(S_+) = S_-$ and vice versa; where

$$S_+ := \{\xi \in S \mid \operatorname{Im} \pi(\xi) > 0\},$$
$$S_- := \{\xi \in S \mid \operatorname{Im} \pi(\xi) < 0\}. \tag{32}$$

That is, S is anti-conformal.

5. Non-negativity of μ

To conclude the proof of Theorem 1 we have to prove that $\mu = \sum_{j=1}^{n} e^{b_j}\delta_{b_j} + \omega \geq 0$. The first summand is obviously non-negative. To prove the second one is also non-negative, we need to show that

$$\omega(s) = \frac{1}{2\pi} \sum_{j:b_j<s} \int_{\partial U} e^{\lambda_j(z)+sz} dz \geq 0; \quad \forall s \in (b_1, b_n]. \tag{33}$$

To do so, we will replace the lift of $\sum_{j:b_j<s} \int_{\partial U}$ on S by $\int_\gamma$ on which the projection of the integrand is real and positive, for some well-chosen contour γ on S.

In the following we fix $s \in (b_k, b_{k+1})$, with $k \in \{1, \ldots, n-1\}$ also fixed. The case $s = b_{k+1}$ is achieved by continuity. We also write $g := \lambda + s\pi$.

5.1. Constructing γ

On S we define $D := \{\xi \mid \frac{\operatorname{Im} g(\xi)}{\operatorname{Im} \pi(\xi)} > 0\}$. For $\xi_0 \in \pi^{-1}(\mathbb{R})$ we note that since the λ_j's have no branch point over $\mathbb{R}$, we locally stay on the same sheet such that π locally has an inverse π^{-1}. Thus, although $\operatorname{Im} \pi(\xi_0) = 0$, we can define the quotient as

$$\frac{\operatorname{Im} g(\xi_0)}{\operatorname{Im} \pi(\xi_0)} := \lim_{y \to 0} \frac{\operatorname{Im} g \circ \pi^{-1}(x_0, y)}{y}, \tag{34}$$

with $\pi(\xi) = x + iy \equiv (x, y)$ and $\pi(\xi_0) = (x_0, 0)$. Furthermore, since $\lambda \circ \pi^{-1}$ is of real type, $\operatorname{Re} g \circ \pi^{-1}(x, y)$ is even in y and hence $(\partial_2 \operatorname{Re} g \circ \pi^{-1})(x_0, 0) = 0$, such that with l'Hôpital's rule we get

$$\frac{\operatorname{Im} g(\xi_0)}{\operatorname{Im} \pi(\xi_0)} = (\partial_2 g \circ \pi^{-1})(x_0, 0); \tag{35}$$

showing that the quotient is well defined for any $\xi \in S$. To help visualize D, we note that $\rho(D) = D$. A possible realization of D is depicted in Figure 2. We next look at $\partial D = \{\xi \mid \frac{\operatorname{Im} g(\xi)}{\operatorname{Im} \pi(\xi)} = 0\}$ and find using equation 35 that $\partial D \cap \pi^{-1}(\mathbb{R})$ is made of discrete points being in fact the continuation of the curves of $\partial D \cap \pi^{-1}(\mathbb{R}^c) = (\operatorname{Im} g)^{-1}(\{0\}) \cap \pi^{-1}(\mathbb{R}^c)$ (see Appendix B of [4]). We propose ∂D to be the trace of γ.

That γ is suited to prove the positivity of μ is the content of

Proposition 5 (The Crucial Link).

$$\frac{1}{2\pi i} \sum_{j:b_j<s} \int_{\partial U} e^{\lambda_j(z)+sz} dz = -\frac{1}{2\pi i} \int_\gamma e^{g(\xi)} d\xi > 0. \tag{36}$$

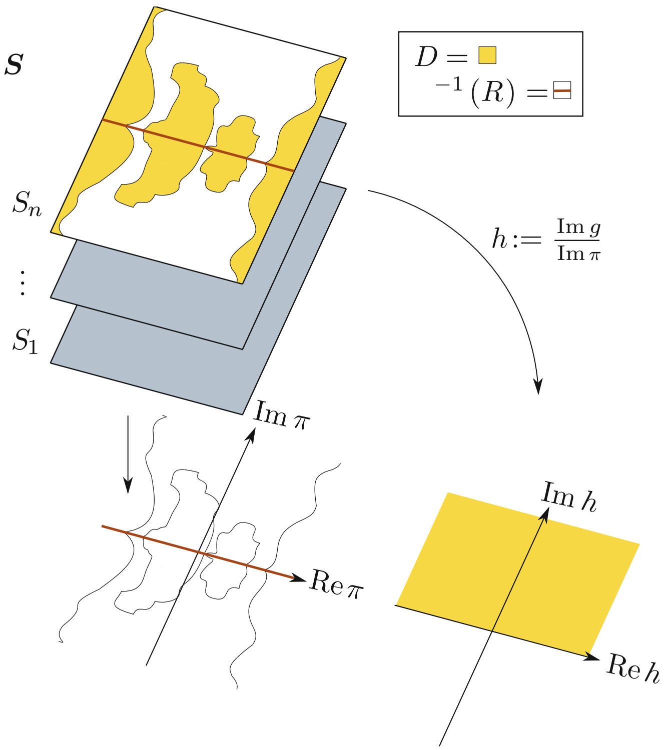

Figure 2. A possible representation of D on S as well as its image through h are displayed in yellow. Note the symmetry of D with respect to $\pi^{-1}(\mathbb{R})$, depicted in brown.

Indeed, proving it concludes the proof of Theorem 1. Before doing so, we though look into some properties of γ.

5.2. Properties of γ

Lemma 6. i) $\gamma = \gamma_1 + \cdots + \gamma_N, \quad \gamma_i$: *positively oriented Jordan curve.*

$$\text{ii)}\quad \operatorname{Re}(g \circ \gamma_k) \quad \begin{array}{l} \textit{monotonically increasing on } \gamma_k^{-1}(S_+), \\ \textit{monotonically decreasing on } \gamma_k^{-1}(S_-). \end{array} \tag{37}$$

Proof. From the above discussion, up to discrete points, the trace of γ is

$$(\operatorname{Im} g)^{-1}(0) \backslash \pi^{-1}(\mathbb{R}).$$

Since $\operatorname{Im} g$ is a harmonic function, everywhere except at a finite number of critical points denoted by C_r, ∂D is locally the trace of a unique curve (see Appendix C of [4] for a proof). Furthermore, since $\operatorname{Im} g$ is non-constant, any point of C_r is found to be a zero of order $m < \infty$ of g; and hence by the auxiliary

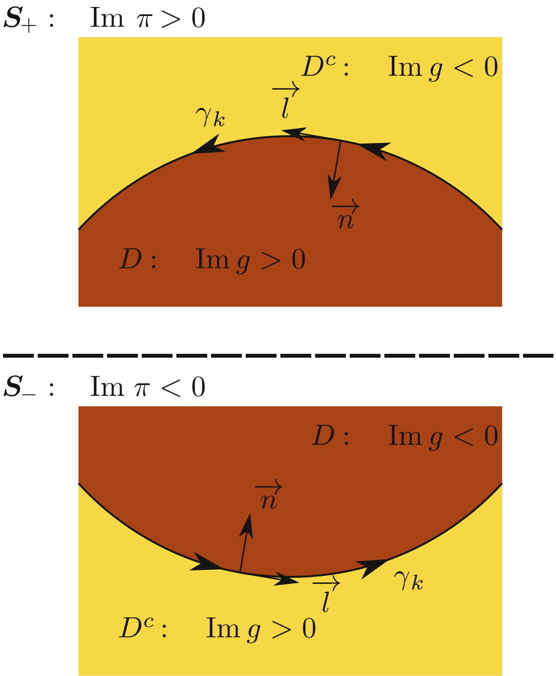

FIGURE 3. The curve γ_k is locally depicted in a region of S_+, top, and S_-, bottom. The change of sign of $\operatorname{Im} g$ is observed when crossing γ_k along the local coordinate $\overrightarrow{n}$.

theorem of Section 4.1 in [10], ∂D is the trace of exactly m curves around such points. Because of the anti-conformal structure of S, those traces form closed loops; allowing us to choose γ as in i).

As depicted in Figure 3, $\operatorname{Im} g$ changes sign when one crosses the trace of γ_k. Choosing the axis l along γ_k and n normal to it pointing in D, this means

$$\begin{aligned} \frac{\partial}{\partial n} \operatorname{Im} g(\xi) > 0 \quad \forall \xi \in \gamma \cap S_+, \\ \frac{\partial}{\partial n} \operatorname{Im} g(\xi) < 0 \quad \forall \xi \in \gamma \cap S_-, \end{aligned} \tag{38}$$

which using the Cauchy–Riemann equations gives

$$\begin{aligned} \frac{\partial}{\partial l} \operatorname{Re} g(\xi) > 0 \quad \forall \xi \in \gamma \cap S_+, \\ \frac{\partial}{\partial l} \operatorname{Re} g(\xi) < 0 \quad \forall \xi \in \gamma \cap S_-; \end{aligned} \tag{39}$$

proving ii). □

Remark 7. Since the γ_k's are single-valued, point ii) of Lemma 6 tells us that each γ_k has to be contained in both S_+ and S_-, allowing us to chose γ such that the endpoints of γ_k lie on $\pi^{-1}(\mathbb{R})$ and $\rho(\gamma_k) = -\gamma_k$.

Lemma 8. $-\frac{1}{2\pi i}\int_{\gamma_k} e^{g(\xi)} d\xi > 0.$

Proof. As $\gamma_k \subset (\operatorname{Im} g)^{-1}(\{0\})$, we have that

$$\operatorname{Im} g(\xi) = 0 \quad \forall \xi \in \gamma_k; \tag{40}$$

and hence together with Lemma 6 ii)

$$e^{g\circ\gamma_k} = e^{\operatorname{Re} g\circ\gamma_k} \text{ is monotonically increasing on } \gamma_k^{-1}(S_+). \tag{41}$$

Writing $z = x + iy$ and $\pi^{-1}(z) = \xi = \nu + i\eta$, we therefore get:

$$\begin{aligned}
\frac{1}{2\pi i}\int_{\gamma_k} e^{g(\xi)} d\xi &= \frac{1}{2\pi i}\left(\int_{\gamma_k\cap S_+} e^{g(\xi)} d\xi + \int_{\gamma_k\cap S_-} e^{g(\xi)} d\xi\right)\\
&\overset{\text{Rem.7}}{=} \frac{1}{2\pi i}\left(\int_{\gamma_k\cap S_+} e^{g(\xi)}(d\nu + id\eta) + \int_{-\gamma_k\cap S_+} e^{\overline{g(\xi)}}(d\nu - id\eta)\right)\\
&\overset{\text{equ.40}}{=} \frac{1}{\pi}\int_{\gamma_k\cap S_+} e^{g(\xi)} d\eta\\
&= \frac{1}{\pi}\int_{\gamma_k^{-1}(S_+)} e^{g\circ\gamma_k(s)} \operatorname{Im}(\pi_\lambda\circ\gamma_k)' ds\\
&\overset{\text{IBP}}{=} -\frac{1}{\pi}\int_{\gamma_k^{-1}(S_+)} \underbrace{\left(e^{g\circ\gamma_k(s)}\right)'}_{>0} \underbrace{\operatorname{Im}(\pi_\lambda\circ\gamma_k)}_{>0} ds < 0,
\end{aligned} \tag{42}$$

where the boundary terms when performing the integration by parts (IBP) vanish because of Remark 7. □

5.3. Proof of the crucial link

We finally prove Proposition 5, which finishes the proof of Theorem 1.

Proof of Proposition 5. From Theorem 2, we can choose a neighborhood of infinity, U, such that λ has no branch point over $\pi^{-1}\left(\overline{U}\right)$. That means that $\pi^{-1}\left(\overline{U}\right)$ is made of n disjoint components, each fully in one sheet. We can hence write:

$$\pi^{-1}(\partial U) = C_1 \cup \cdots \cup C_n\ ; \quad C_j \subset S_j, \quad \forall j = 1, \ldots, n. \tag{43}$$

In $\overline{U}$ we furthermore have by Theorem 2 ii) that

$$\operatorname{Im}(\lambda_j(z) + sz) = (s - b_j)\operatorname{Im}(z) + \operatorname{Im}\left(\mathcal{O}\left(\frac{1}{z}\right)\right). \tag{44}$$

So since $s \in (b_k, b_{k+1})$, for $|z| > R$, $R > 0$ big enough we achieve:

$$\begin{aligned}
j \le k: &\quad \operatorname{Im}(\lambda_j(z) + sz) \text{ has same sign as } \operatorname{Im}(z),\\
j > k: &\quad \operatorname{Im}(\lambda_j(z) + sz) \text{ has opposite sign as } \operatorname{Im}(z).
\end{aligned} \tag{45}$$

Choosing $\overline{U} \subset \{z \mid |z| > R\}$ we have:

$$\begin{aligned} &C_1, \ldots, C_k &&\in D, \\ &C_{k+1}, \ldots, C_n &&\notin D. \end{aligned} \tag{46}$$

Defining $D_0 := D \setminus \pi^{-1}(\overline{U})$, we find with the above $\partial D_0 = \gamma + C_1 + \cdots + C_k$ and, since D_0 is bounded, by Cauchy's Theorem

$$\frac{1}{2\pi i} \int_{\partial D_0} e^{g(\xi)} d\xi = 0; \tag{47}$$

that is

$$\begin{aligned} -\frac{1}{2\pi i} \int_{\gamma} e^{g(\xi)} d\xi &= \frac{1}{2\pi i} \sum_{j=1}^{k} \int_{C_j} e^{\lambda(\xi)+s\pi(\xi)} d\xi = \frac{1}{2\pi i} \sum_{j=1}^{k} \int_{\partial U} e^{\lambda_j(z)+sz} dz \\ &= \frac{1}{2\pi i} \sum_{j : b_j < s} \int_{\partial U} e^{\lambda_j(z)+sz} dz, \end{aligned} \tag{48}$$

which together with Lemma 8 proves the assertion. □

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Some Estimates Regarding Integrated Density of States for Random Schrödinger Operator with Decaying Random Potentials

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Abstract. We investigate some bounds for the integrated density of states in the pure point regime for the random Schrödinger operators with decaying random potentials, given by

$$H^\omega = -\Delta + \sum_{n\in\mathbb{Z}^d} a_n q_n(\omega),$$

acting on $\ell^2(\mathbb{Z}^d)$, where $\{q_n\}_{n\in\mathbb{Z}^d}$ are i.i.d. random variables and $0 < a_n \simeq |n|^{-\alpha},\ \alpha > 0$.

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1. Introduction

The random Schrödinger operator H^ω with decaying randomness on the Hilbert space $\ell^2(\mathbb{Z}^d)$ is given by

$$H^\omega = -\Delta + V^\omega,\ \omega \in \Omega. \tag{1.1}$$

Δ is the adjacency operator defined by

$$(\Delta u)(n) = \sum_{|m-n|=1} u(m)\ \forall\ u \in \ell^2(\mathbb{Z}^d)$$

and

$$V^\omega = \sum_{n\in\mathbb{Z}^d} a_n q_n(\omega) |\delta_n\rangle\langle\delta_n|, \tag{1.2}$$

is the multiplication operator on $\ell^2(\mathbb{Z}^d)$ by the sequence $\{a_n q_n(\omega)\}_{n\in\mathbb{Z}^d}$. Here $\{\delta_n\}_{n\in\mathbb{Z}^d}$ is the standard basis for $\ell^2(\mathbb{Z}^d)$, $\{a_n\}_{n\in\mathbb{Z}^d}$ is a sequence of positive real numbers such that $a_n \to 0$ as $|n| \to \infty$ and $\{q_n\}_{n\in\mathbb{Z}^d}$ are real-valued iid random variables with an absolutely continuous probability distribution μ with bounded density. Here we consider the probability space $\big(\mathbb{R}^{\mathbb{Z}^d}, \mathcal{B}_{\mathbb{R}^{\mathbb{Z}^d}}, \mathbb{P}\big)$, where $\mathbb{P} = \bigotimes \mu$ constructed via the Kolmogorov theorem. We refer to this probability space as $(\Omega, \mathcal{B}, \mathbb{P})$ and $\omega = \big(q_n(\omega)\big)_{n\in\mathbb{Z}^d} \in \Omega$.

For any $B \subset \mathbb{Z}^d$ we consider the canonical orthogonal projection χ_B onto $\ell^2(B)$ and define the matrices

$$\begin{aligned} H_B^\omega &= \big(\langle \delta_n, H^\omega \delta_m\rangle\big)_{n,m\in B}, \quad G^B(z;n,m) = \langle \delta_n, (H_B^\omega - z)^{-1}\delta_m\rangle \\ G^B(z) &= (H_B^\omega - z)^{-1}. \\ G(z) &= (H^\omega - z)^{-1}, \quad G(z;n,m) = \langle \delta_n, (H^\omega - z)^{-1}\delta_m\rangle, z \in \mathbb{C}^+. \end{aligned} \tag{1.3}$$

Note that H_B^ω is the matrix

$$H_B^\omega = \chi_B H^\omega \chi_B \ : \ \ell^2(B) \longrightarrow \ell^2(B), \ a.e.\ \omega.$$

One can note that the operators $\{H^\omega\}_{\omega\in\Omega}$ are self-adjoint a.e. ω and have a common core domain consisting of vectors with finite support.

Let Λ_L denote the d-dimension box:

$$\Lambda_L = \{(n_1, n_2, \cdots, n_d) \in \mathbb{Z}^d : |n_i| \le L\} \subset \mathbb{Z}^d.$$

We will work with the following hypothesis:

Hypothesis 1.1.

(1) *The measure μ is absolute continuous and the density of μ is given by*

$$\rho(x) = \begin{cases} 0 & \text{if } |x| < 1 \\ \frac{\delta-1}{2}\,\frac{1}{|x|^\delta} & \text{if } |x| \ge 1, \text{ for some } \delta > 1. \end{cases} \tag{1.4}$$

(2) *The sequence a_n satisfies $a_n \simeq |n|^{-\alpha}$, $\alpha > 0$.*

(3) *The pair (α, δ) is chosen such that $d - \alpha(\delta - 1) > 0$ holds. This implies that $\beta_L \to \infty$ as $L \to \infty$, where β_L is given by*

$$\beta_L = \sum_{n\in\Lambda_L} a_n^{\delta-1} \simeq \sum_{n\in\Lambda_L} |n|^{-\alpha(\delta-1)} = O\Big((2L+1)^{d-\alpha(\delta-1)}\Big). \tag{1.5}$$

Remark 1.2. We have taken an explicit $\rho(x)$ in (1.4) in order to simplify the calculations in the proofs. Our results also hold for $\rho(x) = O\big(\frac{1}{|x|^\delta}\big)$, $\delta > 1$ as $|x| \to \infty$.

In [21], Kirsch–Krishna–Obermeit consider $H^\omega = -\Delta + V^\omega$ on $\ell^2(\mathbb{Z}^d)$ with the same V^ω as defined in (1.2). They showed that $\sigma(H^\omega) = \mathbb{R}$ and $\sigma_c(H^\omega) \subseteq [-2d, 2d]$ a.e. ω, under some conditions on $\{a_n\}_{n\in\mathbb{Z}^d}$ and μ (The density of μ should not decay too fast at infinity and a_n should not decay too fast). For the precise condition on a_n's and μ we recall Definition 2.1 from [21], which is given as follows.

Definition 1.3. Let $\{a_n\}$ be a bounded, positive sequence on $\mathbb{R}$. Then, $\{a_n\}$ – supp μ is defined by

$$\{a_n\} - \text{supp } \mu := \Big\{x \in \mathbb{R} : \sum_n \mu\big(a_n^{-1}(x-\epsilon, x+\epsilon)\big) = \infty \ \forall\ \epsilon > 0\Big\}. \tag{1.6}$$

We call a probability measure μ asymptotically large with respect to a_n if $\{a_{kn}\}$ – supp $\mu = \mathbb{R}$, for all $k \in \mathbb{Z}^+$.

To show the existence of point spectrum outside $[-2d, 2d]$ they verified Simon-Wolf criterion [25, Theorem 12.5] by showing exponential decay of the fractional moment of the Green function [21, Lemma 3.2]. The decay is valid for $|n-m| > 2R$ with energy $E \in \mathbb{R} \setminus [-2d, 2d]$ and is given by

$$\mathbb{E}^\omega(|G^{\Lambda_L}(E+i\epsilon : n, m)|^s) \leq D_{P(n.m)} e^{-c\left(\frac{|n-m|}{2}\right)},\ E \in \mathbb{R} \setminus [-2d, 2d], \tag{1.7}$$

where $\epsilon > 0$, $0 < s < 1$, c is a positive constant independent of ϵ and if E is in compact interval then we can also choose c independent of E. Here $R \in \mathbb{Z}^+$ and $D_{P(n.m)}$ is a constant independent of E and ϵ, but polynomially bounded in $|n|$ and $|m|$.

Jakšić–Last showed in [15, Theorem 1.2] that for $d \geq 3$, if $a_n \simeq |n|^{-\alpha}$ $\alpha > 1$ then there is no singular spectrum inside $(-2d, 2d)$ of H^ω.

Here we take (a_n, μ) such that $\{a_{kn}\}$ – supp $\mu = \mathbb{R}$ for each $k \in \mathbb{Z}^+$ and satisfying Hypothesis 1.1. Then it follows from [21, Theorem 2.7] that the spectrum of H^ω is $\mathbb{R}$ and $\sigma_c(H^\omega) \subseteq [-2d, 2d]$ a.e. ω. We show that the average spacing of eigenvalues of $H^\omega_{\Lambda_L}$ near the energy $E \in \mathbb{R} \setminus [-2d, 2d]$ are of order β_L^{-1}, whereas those close to $E \in [-2d, 2d]$ have average spacing of the order $\frac{1}{(2L+1)^d}$. This shows that the eigenvalues of $H^\omega_{\Lambda_L}$ are more densely distributed inside $[-2d, 2d]$, where the continuous part of the spectrum of H^ω lies, than the pure point regime which is outside $[-2d, 2d]$.

We need the following definitions before stating the results:

$$N^\omega_L(E) = \#\{j : E_j \leq E,\ E_j \in \sigma(H^\omega_{\Lambda_L})\}, \tag{1.8}$$

$$\tilde{N}^\omega_L(E) = \#\{j : E_j \geq E,\ E_j \in \sigma(H^\omega_{\Lambda_L})\}, \tag{1.9}$$

$$\gamma_L(\cdot) = \frac{1}{\beta_L} \sum_{n \in \Lambda_L} \mathbb{E}^\omega\big(\langle \delta_n, E_{H^\omega_{\Lambda_L}}(\cdot)\delta_n\rangle\big). \tag{1.10}$$

In the above $E_{H^\omega_{\Lambda_L}}(\cdot)$ denotes the spectral projection of $H^\omega_{\Lambda_L}$.

Our main results are as follows:

Theorem 1.4. *If $E < -2d$ and $\epsilon = -2d - E > 0$ then, we have*

$$\frac{1}{2}\frac{1}{(4d+\epsilon)^{(\delta-1)}} \leq \varliminf_{L\to\infty} \frac{1}{\beta_L}\mathbb{E}^\omega(N^\omega_L(E)) \leq \varlimsup_{L\to\infty} \frac{1}{\beta_L}\mathbb{E}^\omega(N^\omega_L(E)) \leq \frac{1}{2}\frac{1}{\epsilon^{(\delta-1)}}.$$

For $E = 2d + \epsilon > 2d$ we have

$$\frac{1}{2}\frac{1}{(4d+\epsilon)^{(\delta-1)}} \leq \varliminf_{L\to\infty} \frac{1}{\beta_L}\mathbb{E}^\omega(\tilde{N}^\omega_L(E)) \leq \varlimsup_{L\to\infty} \frac{1}{\beta_L}\mathbb{E}^\omega(\tilde{N}^\omega_L(E)) \leq \frac{1}{2}\frac{1}{\epsilon^{(\delta-1)}}.$$

Now we investigate the average number of eigenvalues of $H^{\omega}_{\Lambda_L}$ inside $[-2d, 2d]$, which can be given as follows:

Corollary 1.5. *For any interval $I \supsetneq [-2d, 2d]$ we have*

$$\lim_{L\to\infty} \frac{1}{(2L+1)^d} \mathbb{E}^{\omega}\big(\#\{\sigma(H^{\omega}_{\Lambda_L}) \cap I\}\big) = 1. \tag{1.11}$$

Corollary 1.6. *If $M_1 < -2d$ and $M_2 > 2d$ then, we have*

$$\overline{\lim_{L\to\infty}}\, \gamma_L\big((-\infty, M_1] \cup [M_2, \infty)\big) \leq \frac{1}{2}\left[\frac{1}{(-2d - M_1)^{(\delta-1)}} + \frac{1}{(M_2 - 2d)^{(\delta-1)}}\right]. \tag{1.12}$$

For any interval $I \subseteq \mathbb{R} \setminus [-2d, 2d]$ of length $|I| > 4d$ there is a constant $C_I > 0$ such that

$$\underline{\lim_{L\to\infty}}\, \gamma_L(I) \geq C_I > 0. \tag{1.13}$$

Corollary 1.7. *Let $M_1 < -2d$ and $M_2 > 2d$ and $\gamma_L \restriction_{(M_1,M_2)^c}$ denote the restriction of γ_L to $\mathbb{R} \setminus (M_1, M_2)$. The sequence of measure $\{\gamma_L \restriction_{(M_1,M_2)^c}\}_L$ admits a subsequence which converges vaguely to a non-trivial measure, say γ.*

The above theorem gives estimates for the average of $N^{\omega}_L(E)$ and $\tilde{N}^{\omega}_L(E)$, but we can also get a point-wise estimate of the above quantities which is given by the following theorem.

Theorem 1.8. *For $d \geq 2$, $0 < \alpha < \frac{1}{2}$ and $1 < \delta < \frac{1}{2\alpha}$ then for almost all ω*

$$\begin{aligned}
\frac{1}{2}\frac{1}{(2d-E)^{(\delta-1)}} &\leq \underline{\lim_{L\to\infty}}\, \frac{1}{\beta_L} N^{\omega}_L(E) \leq \overline{\lim_{L\to\infty}}\, \frac{1}{\beta_L} N^{\omega}_L(E)\\
&\leq \frac{1}{2}\frac{1}{(-2d-E)^{(\delta-1)}} \quad \textit{for } E < -2d,\\
\frac{1}{2}\frac{1}{(2d+E)^{(\delta-1)}} &\leq \underline{\lim_{L\to\infty}}\, \frac{1}{\beta_L} \tilde{N}^{\omega}_L(E) \leq \overline{\lim_{L\to\infty}}\, \frac{1}{\beta_L} \tilde{N}^{\omega}_L(E)\\
&\leq \frac{1}{2}\frac{1}{(E-2d)^{(\delta-1)}} \quad \textit{for } E > 2d.
\end{aligned}$$

In [11], Figotin–Germinet–Klein–Müller studied the Anderson Model on $L^2(\mathbb{R}^d)$ with decaying random potentials given by

$$H^{\omega} = -\Delta + \lambda\gamma_{\alpha}V^{\omega} \ \textit{on}\ L^2(\mathbb{R}^d),$$

where $\lambda > 0$ is the disorder parameter and γ_{α} is the envelope function

$$\gamma_{\alpha}(x) := (1 + |x|^2)^{-\frac{\alpha}{2}},\ \alpha \geq 0.$$

They assumed that the density of the single site distribution is a compact supported L^{∞} function. They showed that for $\alpha \in (0, 2)$ the operator H^{ω} has infinitely many eigenvalues in $(-\infty, 0)$ a.e. ω. In [11, Theorem 3], they gave the bound for $N^{\omega}(E)$, $E < 0$ (number of eigenvalues of H^{ω} below E) in terms of density of states for the stationary (i.i.d. case) model.

In [14], Gordon–Jaksić–Molchanov–Simon studied the model given by

$$H^\omega = -\Delta + \sum_{n\in\mathbb{Z}^d} (1+|n|^\alpha) q_n(\omega),\ \ \alpha > 0 \ \mathit{on}\ \ell^2(\mathbb{Z}^d),$$

where $\{q_n\}$ are i.i.d. random variables uniformly distributed on $[0,1]$. They showed that if $\alpha > d$ then H^ω has discrete spectrum a.e. ω. For the case when $\alpha \leq d$ they construct a strictly decreasing sequence $\{a_k\}_{k\in\mathbb{N}}$ of positive numbers such that if $\frac{d}{k} \geq \alpha > \frac{d}{k+1}$ then for a.e. ω we have the following:

(i) $\sigma(H^\omega) = \sigma_{pp}(H^\omega)$ and the eigenfunctions of H^ω decay exponentially,
(ii) $\sigma_{\text{ess}}(H^\omega) = [a_k, \infty)$ and
(iii) $\#\sigma_{\text{disc}}(H^\omega) < \infty$.

They also showed that

(a) If $\frac{d}{k} > \alpha > \frac{d}{k+1}$ and $E \in (a_j, a_{j-1})$, $1 \leq j \leq k$, then
$$\lim_{L\to\infty} \frac{N_L^\omega(E)}{L^{d-j\alpha}} = N_j(E)$$
exists for a.e. ω and is a non-random function.

(b) If $\alpha = \frac{d}{k}$ and $E \in (a_j, a_{j-1})$, $1 \leq j < k$ the above is valid. If $E \in (a_k, a_{k-1})$ then
$$\lim_{L\to\infty} \frac{N_L^\omega(E)}{lnL} = N_k(E)$$
exists for a.e. ω and is a non-random function.

Böcker in his doctoral thesis [4] showed the strong law of large numbers for sparse random potentials. He also studied the density of surface states for some non-stationary potentials. Using a Laplace transform they studied the asymptotic behaviour of the integrated density of surface states for random Gaussian surface potentials.

In [5] Böcker–Werner–Stollmann review some recent results on the spectral theory of non-stationary random potentials. They present various models with decaying and sparse random potentials, including those where the sparse set itself is random. Their results include a definition of the integrated density of states and some results on Lifshits tails for such models.

In this work, we essentially show that for decaying potentials the confinement length is $(2L+1)^d$ inside $[-2d, 2d]$ and β_L outside $[-2d, 2d]$. On the other hand, for the growing potentials (as in [14]), the confinement length is a function of energy.

2. On the pure point and continuous spectrum

In this section, we work out the spectrum of H^ω under the Hypothesis 1.1. Here we use [21, Corollary 2.5] and [21, Theorem 2.3].

Let $x < 0$ and $\epsilon > 0$ such that $x + \epsilon < 0$ then, for large enough $|n| \geq M$ we have $a_n^{-1}(x+\epsilon) \leq -1$ since $a_n^{-1} \to \infty$ as $|n| \to \infty$.

For $|n| \geq M$ we have

$$\mu\bigg(\frac{1}{a_n}(x-\epsilon, x+\epsilon)\bigg) = \int_{a_n^{-1}(x-\epsilon)}^{a_n^{-1}(x+\epsilon)} \rho(t)dt = a_n^{(\delta-1)}\frac{\delta-1}{2}\int_{x-\epsilon}^{x+\epsilon}\frac{1}{|t|^\delta}dt \text{ (using 1.4).}$$

Hence,

$$\sum_{n\in\mathbb{Z}^d}\mu\bigg(\frac{1}{a_n}(x-\epsilon, x+\epsilon)\bigg) \geq \frac{\delta-1}{2}\int_{x-\epsilon}^{x+\epsilon}\frac{1}{|t|^\delta}dt\sum_{|n|\geq M} a_n^{(\delta-1)} = \infty, \tag{2.1}$$

since $\beta_L = \sum_{n\in\Lambda_L} a_n^{(\delta-1)} \to \infty$ as $L \to \infty$ (using 1.5).

For $x > 0$, a similar calculation will give

$$\sum_{n\in\mathbb{Z}^d}\mu\bigg(\frac{1}{a_n}(x-\epsilon, x+\epsilon)\bigg) = \infty, \ \epsilon > 0. \tag{2.2}$$

Now let $\epsilon > 0$, there exist M such that $a_n^{-1}\epsilon > 1$ for $|n| \geq M$. So, we have

$$\begin{aligned}\sum_{n\in\mathbb{Z}^d}\mu\bigg(\frac{1}{a_n}(-\epsilon, \epsilon)\bigg) &\geq \sum_{|n|\geq M}\mu(-a_n^{-1}\epsilon, a_n^{-1}\epsilon) = 2\sum_{|n|\geq M}\frac{\delta-1}{2}\int_1^{a_n^{-1}\epsilon}\frac{1}{t^\delta}dt \\ &= \sum_{|n|\geq M}(1-\epsilon^{1-\delta}a_n^{\delta-1}).\end{aligned}$$

Since

$$\sum_{n\in\Lambda_L}(1-\epsilon^{1-\delta}a_n^{\delta-1}) \approx \big[(2L+1)^d - (2L+1)^{d-\alpha(\delta-1)}\big] \to \infty \quad \text{as } L \to \infty,$$

it follows that

$$\sum_{n\in\mathbb{Z}^d}\mu\bigg(\frac{1}{a_n}(-\epsilon, \epsilon)\bigg) = \infty. \tag{2.3}$$

If $0 < \epsilon_1 < \epsilon_2$, then we have

$$\mu\Big(a_n^{-1}(x-\epsilon_1, x+\epsilon_1)\Big) \leq \mu\Big(a_n^{-1}(x-\epsilon_2, x+\epsilon_2)\Big) \ \forall \ x \in \mathbb{R}.$$

Using the above inequality together with (2.1), (2.2) and (2.3) we have

$$\sum_{n\in\mathbb{Z}^d}\mu\Big(a_n^{-1}(x-\epsilon, x+\epsilon)\Big) = \infty, \text{ for all } x \in \mathbb{R} \ \& \ \epsilon > 0. \tag{2.4}$$

Then, using (2.4) from [21, Definition 2.1], we see that

$$M = \cap_{k\in\mathbb{Z}^+}(a_{kn} - \text{supp } \mu) = \mathbb{R}.$$

Therefore, [21, Corollary 2.5] and [21, Theorem 2.3] will give the following description about the spectrum of H^ω.

$$\sigma_{\text{ess}}(H^\omega) = [-2d, 2d] + \mathbb{R} = \mathbb{R} \ \textit{and} \ \sigma_c(H^\omega) \subseteq [-2d, 2d] \ \textit{a.e} \ \omega.$$

3. Proof of main results

Proof of Theorem 1.4. Define

$$A^{\omega}_{L,\pm} = \pm 2d + \sum_{n\in\Lambda_L} a_n q_n(\omega) P_{\delta_n}$$

and

$$N^{\omega}_{\pm,L}(E) = \#\{j;\ E_j \leq E,\ E_j \in \sigma(A^{\omega}_{L,\pm})\},$$
$$N^{\omega}_{L}(E) = \#\{j : E_j \leq E,\ E_j \in \sigma(H^{\omega}_{\Lambda_L})\}.$$

Since $\sigma(\Delta) = [-2d, 2d]$, the following operator inequality

$$A^{\omega}_{L,-} \leq H^{\omega}_{\Lambda_L} \leq A^{\omega}_{L,+} \tag{3.1}$$

is there, with

$$H^{\omega}_{\Lambda_L} = \chi_{\Lambda_L}\Delta\chi_{\Lambda_L} + \sum_{n\in\Lambda_L} a_n q_n(\omega) P_{\delta_n}.$$

A simple application of the min-max principle [16, Theorem 6.44] shows that

$$N^{\omega}_{+,L}(E) \leq N^{\omega}_{L}(E) \leq N^{\omega}_{-,L}(E). \tag{3.2}$$

Now, the spectrum $\sigma(A^{\omega}_{L,\pm})$ of $A^{\omega}_{L,\pm}$ consists of only eigenvalues and is given by

$$\sigma(A^{\omega}_{L,\pm}) = \{n \in \Lambda_L : \pm 2d + a_n q_n(\omega)\}.$$

Let $E < -2d$ with $E = -2d - \epsilon$, for some $\epsilon > 0$. Then,

$$\begin{aligned} N^{\omega}_{-,L}(E) &= \#\{n \in \Lambda_L : -2d + a_n q_n(\omega) \leq -2d - \epsilon\} \\ &= \#\{n \in \Lambda_L : q_n(\omega) \in (-\infty, -a_n^{-1}\epsilon]\} \\ &= \sum_{n\in\Lambda_L} \chi_{\{\omega : q_n(\omega)\in(-\infty,-a_n^{-1}\epsilon]\}}. \end{aligned} \tag{3.3}$$

Since q_n are i.i.d, if we take expectation of both sides of (3.3) we get

$$\mathbb{E}^{\omega}(N^{\omega}_{-,L}(E)) = \sum_{n\in\Lambda_L} \mu(-\infty, -a_n^{-1}\epsilon] = \sum_{n\in\Lambda_L} \int_{-\infty}^{-a_n^{-1}\epsilon} \rho(x)dx. \tag{3.4}$$

Since $a_n^{-1} \to \infty$ as $|n| \to \infty$ and $\epsilon > 0$, there exist an $M \in \mathbb{N}$ such that

$$a_n^{-1}\epsilon > 1,\ -a_n^{-1}\epsilon < -1\ \forall\ |n| > M.$$

Therefore for large L, from (3.3) we get

$$\begin{aligned} \mathbb{E}^{\omega}(N^{\omega}_{-,L}(E)) &= \sum_{n\in\Lambda_L} \int_{-\infty}^{-a_n^{-1}\epsilon} \rho(x)dx \\ &= \sum_{n\in\Lambda_L,\ |n|>M} \int_{-\infty}^{-a_n^{-1}\epsilon} \rho(x)dx + \sum_{n\in\Lambda_L,\ |n|\leq M} \int_{-\infty}^{-1} \rho(x)dx. \end{aligned} \tag{3.5}$$

Since $\#\{n \in \mathbb{Z}^d : |n| \leq M\} \leq (2M+1)^d$, we have

$$\sum_{n\in\Lambda_L,\ |n|\leq M} \int_{-\infty}^{-1} \rho(x)dx \leq (2M+1)^d \int_{-\infty}^{-1} \rho(x)dx = (2M+1)^d\ \frac{\delta-1}{2} \int_{-\infty}^{-1} \frac{1}{|x|^\delta}dx$$
$$= (2M+1)^d \big/ 2,\ \ \delta > 1 \text{ is given.} \tag{3.6}$$

Using (1.5) on (3.6) we have

$$\lim_{L\to\infty} \frac{1}{\beta_L} \sum_{n\in\Lambda_L,\ |n|\leq M} \int_{-\infty}^{-1} \rho(x)dx = 0. \tag{3.7}$$

Now,

$$\sum_{n\in\Lambda_L,\ |n|>M} \int_{-\infty}^{-a_n^{-1}\epsilon} \rho(x)dx = \sum_{n\in\Lambda_L,\ |n|>M} a_n^{-1} \int_{-\infty}^{-\epsilon} \rho(a_n^{-1}t)dt \tag{3.8}$$
$$= \sum_{n\in\Lambda_L,\ |n|>M} a_n^{(\delta-1)} \frac{\delta-1}{2} \int_{-\infty}^{-\epsilon} \frac{1}{|t|^\delta}dt = \frac{\epsilon^{1-\delta}}{2} \sum_{n\in\Lambda_L,\ |n|>M} a_n^{(\delta-1)},\ \ \delta > 1.$$

This equality gives

$$\lim_{L\to\infty} \frac{1}{\beta_L} \sum_{n\in\Lambda_L,\ |n|>M} \int_{-\infty}^{-a_n^{-1}\epsilon} \rho(x)dx = \frac{\epsilon^{1-\delta}}{2}. \tag{3.9}$$

Using (3.7) and (3.9) in (3.5), we have

$$\lim_{L\to\infty} \frac{1}{\beta_L}\mathbb{E}^\omega(N^\omega_{-,L}(E)) = \frac{\epsilon^{1-\delta}}{2} = \frac{1}{2\ \epsilon^{(\delta-1)}} > 0. \tag{3.10}$$

A similar calculation with $\mathbb{E}^\omega(N^\omega_{+,L}(E))$ gives,

$$\lim_{L\to\infty} \frac{1}{\beta_L}\mathbb{E}^\omega(N^\omega_{+,L}(E)) = \frac{(4d+\epsilon)^{1-\delta}}{2} = \frac{1}{2\ (4d+\epsilon)^{(\delta-1)}} > 0. \tag{3.11}$$

Now, using (3.10) and (3.11) from (3.2), we conclude the inequality

$$\frac{1}{2}\frac{1}{(4d+\epsilon)^{(\delta-1)}} \leq \varliminf_{L\to\infty} \frac{1}{\beta_L}\mathbb{E}^\omega(N^\omega_L(E)) \leq \varlimsup_{L\to\infty} \frac{1}{\beta_L}\mathbb{E}^\omega(N^\omega_L(E)) \leq \frac{1}{2}\frac{1}{\epsilon^{(\delta-1)}}. \tag{3.12}$$

If we define

$$\begin{aligned} \tilde{N}^\omega_{\pm,L}(E) &= \#\{j : E_j \geq E,\ E_j \in \sigma(A^\omega_{L\pm})\}, \\ \tilde{N}^\omega_L(E) &= \#\{j : E_j \geq E,\ E_j \in \sigma(H^\omega_{\Lambda_L})\} \end{aligned} \tag{3.13}$$

then the min-max theorem and (3.1) together will give

$$\tilde{N}^\omega_{-,L}(E) \leq \tilde{N}^\omega_L(E) \leq \tilde{N}^\omega_{+,L}(E). \tag{3.14}$$

If $E = 2d + \epsilon > 2d$, for some $\epsilon > 0$, a similar calculation results in

$$\frac{1}{2}\frac{1}{(4d+\epsilon)^{(\delta-1)}} \leq \varliminf_{L\to\infty} \frac{1}{\beta_L}\mathbb{E}^\omega(\tilde{N}^\omega_L(E)) \leq \varlimsup_{L\to\infty} \frac{1}{\beta_L}\mathbb{E}^\omega(\tilde{N}^\omega_L(E)) \leq \frac{1}{2}\frac{1}{\epsilon^{(\delta-1)}}. \tag{3.15}$$

The inequalities (3.12) and (3.15) together prove Theorem 1.4. □

Proof of Corollary 1.5. Since $H^\omega_{\Lambda_L}$ is a matrix of order $(2L+1)^d$, we have

$$\#\sigma(H^\omega_{\Lambda_L}) = (2L+1)^d.$$

If $M_1 < -2d$ and $M_2 > 2d$ then,

$$\begin{aligned}\#\Big\{\sigma(H^\omega_{\Lambda_L}) \cap (-\infty, M_1]\Big\} + \#\Big\{\sigma(H^\omega_{\Lambda_L}) \cap (M_1, M_2)\Big\} \\ + \#\Big\{\sigma(H^\omega_{\Lambda_L}) \cap [M_2, \infty)\Big\} = (2L+1)^d.\end{aligned} \tag{3.16}$$

Since

$$\frac{1}{(2L+1)^d}\mathbb{E}^\omega\{\sigma(H^\omega_{\Lambda_L}) \cap (-\infty, M_1]\} = \frac{\beta_L}{(2L+1)^d}\frac{1}{\beta_L}\mathbb{E}^\omega(N^\omega_L(M_1)), \tag{3.17}$$

and from (3.12) and Hypothesis 1.1 we have

$$\overline{\lim_{L\to\infty}} \frac{1}{\beta_L}\mathbb{E}^\omega(N^\omega_L(M_1)) < \infty, \quad \text{and } \lim_{L\to\infty} \frac{\beta_L}{(2L+1)^d} = 0,$$

the following limit holds:

$$\lim_{L\to\infty} \frac{1}{(2L+1)^d}\mathbb{E}^\omega\{\sigma(H^\omega_{\Lambda_L}) \cap (-\infty, M_1]\} = 0. \tag{3.18}$$

Similarly, using (3.15) we get

$$\lim_{L\to\infty} \frac{1}{(2L+1)^d}\mathbb{E}^\omega\{\sigma(H^\omega_{\Lambda_L}) \cap [M_2, \infty)\} = 0. \tag{3.19}$$

Using the inequalities (3.16), (3.18) and (3.19), we see that for any interval (M_1, M_2) containing $[-2d, 2d]$

$$\lim_{L\to\infty} \frac{1}{(2L+1)^d}\mathbb{E}^\omega\big(\#\{\sigma(H^\omega_{\Lambda_L}) \cap (M_1, M_2)\}\big) = 1. \qquad \square$$

Proof of Corollary 1.6. If $M_1 < -2d$ then from (1.10) we have

$$\begin{aligned}\gamma_L(-\infty, M_1] &= \frac{1}{\beta_L}\mathbb{E}^\omega\Big(Tr\big(E_{H^\omega_{\Lambda_L}}(-\infty, M_1]\big)\Big) \\ &= \frac{1}{\beta_L}\mathbb{E}^\omega\big(N^\omega_L(M_1)\big) \qquad \text{(using (1.8))}.\end{aligned} \tag{3.20}$$

This equality together with (3.12) gives

$$\overline{\lim_{L\to\infty}}\, \gamma_L(-\infty, M_1] \leq \frac{1}{2\ (-2d - M_1)^{\delta-1}} \qquad (\text{using } \epsilon = -2d - M_1). \tag{3.21}$$

Similarly, for $M_2 > 2d$, using (3.15), we get

$$\overline{\lim_{L\to\infty}}\, \gamma_L[M_2, \infty) \leq \frac{1}{2\ (M_2 - 2d)^{\delta-1}} \ (\text{using } \epsilon = M_2 - 2d). \tag{3.22}$$

(3.21) and (3.22) together proves (1.12).

Let $J = [E_1, E_2] \subset (-\infty, -2d)$ with $|J| > 4d$, set $E_1 = -2d - \epsilon_1$, $E_2 = -2d - \epsilon_2$ such that $\epsilon_1 - \epsilon_2 > 4d$. Then

$$\begin{aligned}\gamma_L(J) &= \frac{1}{\beta_L}\mathbb{E}^\omega\big(N_L^\omega(E_2)\big) - \frac{1}{\beta_L}\mathbb{E}^\omega\big(N_L^\omega(E_1)\big) \\ &\geq \frac{1}{\beta_L}\mathbb{E}^\omega\big(N_{+,L}^\omega(E_2)\big) - \frac{1}{\beta_L}\mathbb{E}^\omega\big(N_{-,L}^\omega(E_1)\big) \text{ (using (3.2)).}\end{aligned} \tag{3.23}$$

Therefore, (3.11) and (3.10) give (1.13), namely

$$\varliminf_{L\to\infty} \gamma_L(J) \geq \frac{1}{2}\left[\frac{1}{(4d+\epsilon_2)^{(\delta-1)}} - \frac{1}{\epsilon_1^{(\delta-1)}}\right] > 0.$$

A similar result holds even when $J \subset (2d, \infty)$ with $|J| > 4d$. □

Proof of Corollary 1.7. From (1.12) we have

$$\sup_L \gamma_L\big((-\infty, M_1] \cup [M_2, \infty)\big) < \infty. \tag{3.24}$$

We write $\mathbb{R} \setminus (M_1, M_2) = \bigcup_n A_n$, countable union of compact sets. Now, $\gamma_L \restriction_{A_n}$ (restriction of γ_L to A_n) admits a weakly convergence subsequence by the Banach–Alaoglu Theorem. Then, by a diagonal argument we select a subsequence of $\{\gamma_L\}$ which converges vaguely to a non-trivial measure, say γ on $\mathbb{R} \setminus (M_1, M_2)$.

The non-triviality of γ is given by the fact that if $J \subset \mathbb{R} \setminus (M_1, M_2)$ is an interval such that $4d < |J| < \infty$ then from (1.13) we get

$$\inf_L \gamma_L(J) > 0.$$ □

Before we proceed to the proof of Theorem 1.8, we prove the following lemma.

Lemma 3.1. *Let $\{X_n\}$ be a sequence of random variables on a probability space $\big(\Omega, \mathcal{B}, \mathbb{P}\big)$ satisfying*

$$\sum_{n=1}^{\infty} \mathbb{P}\big(\omega : |X_n(\omega) - X(\omega)| > \epsilon\big) < \infty, \ \epsilon > 0.$$

Then $X_n \xrightarrow{n\to\infty} X$ a.e. ω.

Proof. Define $A_n(\epsilon) = \big\{\omega : |X_n(\omega) - X(\omega)| > \epsilon\big\}$. If

$$\sum_{n=1}^{\infty} \mathbb{P}\big(A_n(\epsilon)\big) = \sum_{n=1}^{\infty} \mathbb{P}\big(\omega : |X_n(\omega) - X(\omega)| > \epsilon\big) < \infty,$$

then the Borel–Cantelli lemma gives

$$\mathbb{P}\big(A(\epsilon)\big) = 0, \text{ where } A(\epsilon) = \bigcap_{n=1}^{\infty} \bigcup_{m=n}^{\infty} A_n(\epsilon).$$

Now we have

$$\mathbb{P}\big(B(\epsilon)\big) = 1 \text{ where } B(\epsilon) = \bigcup_{n=1}^{\infty} \bigcap_{m=n}^{\infty} A_n(\epsilon)^c.$$

For each $N \in \mathbb{N}$, we define

$$B_N = B(1/N) \quad \text{and} \quad B = \bigcap_{N=1}^{\infty} B_N \text{ then } \mathbb{P}(B) = 1, \text{ since } \mathbb{P}(B_N) = 1.$$

For any $\delta > 0$, we can choose $M \in \mathbb{N}$ such that $\frac{1}{M} < \delta$. If $\omega \in B$ then, $\forall\, N \in \mathbb{N}\ \omega \in B_N$. From the construction of B_M, there exists a $K \in \mathbb{N}$ such that

$$|X_m(\omega) - X(\omega)| \le \frac{1}{M} < \delta \ \forall\, m \ge K.$$

So we have

$$X_m \xrightarrow{m\to\infty} X \text{ on } B \text{ with } \mathbb{P}(B) = 1.$$

Hence the lemma. □

Proof of Theorem 1.8. Let $E = -2d - \epsilon$ for some $\epsilon > 0$ and define

$$X_n(\omega) := \chi_{\{\omega : q_n(\omega) \le -a_n^{-1}\epsilon\}}. \tag{3.25}$$

Since $\{q_n\}_n$ are i.i.d., $\{X_n\}$ is a sequence of independent random variables. Now, from (3.3) we have

$$N^{\omega}_{-,L}(E) = \sum_{n\in\Lambda_L} X_n(\omega). \tag{3.26}$$

We want to prove the following:

$$\lim_{L\to\infty} \frac{N^{\omega}_{-,L}(E) - \mathbb{E}^{\omega}\big(N^{\omega}_{-,L}(E)\big)}{\beta_L} = 0 \ a.e\ \omega. \tag{3.27}$$

In view of Lemma 3.1, in order to prove the above equation, it is enough to show

$$\sum_{L=1}^{\infty} \mathbb{P}\left(\omega : \frac{\big|N^{\omega}_{-,L}(E) - \mathbb{E}^{\omega}\big(N^{\omega}_{-,L}(E)\big)\big|}{\beta_L} > \eta\right) < \infty \ \forall\, \eta > 0. \tag{3.28}$$

Using Chebyshev's inequality we get

$$\begin{aligned} &\sum_{L=1}^{\infty} \mathbb{P}\left(\omega : \frac{\big|N^{\omega}_{-,L}(E) - \mathbb{E}^{\omega}\big(N^{\omega}_{-,L}(E)\big)\big|}{\beta_L} > \eta\right) \\ &\quad \le \sum_{L=1}^{\infty} \frac{1}{\eta^2\beta_L^2} \mathbb{E}^{\omega}\Big(N^{\omega}_{-,L}(E) - \mathbb{E}^{\omega}\big(N^{\omega}_{-,L}(E)\big)\Big)^2. \end{aligned} \tag{3.29}$$

We proceed to estimate the RHS of the above inequality.

$$\begin{aligned} \mathbb{E}^{\omega}\Big(N^{\omega}_{-,L}(E) - \mathbb{E}^{\omega}\big(N^{\omega}_{-,L}(E)\big)\Big)^2 &= \mathbb{E}^{\omega}\left(\sum_{n\in\Lambda_L} \big(X_n(\omega) - \mathbb{E}^{\omega}\big(X_n(\omega)\big)\big)\right)^2 \\ &= \sum_{n\in\Lambda_L} \mathbb{E}^{\omega}\Big(X_n(\omega) - \mathbb{E}^{\omega}\big(X_n(\omega)\big)\Big)^2 \quad (X_n \text{ are independent}) \\ &= \sum_{n\in\Lambda_L} \Big[\mathbb{E}^{\omega}(X_n^2) - \big(\mathbb{E}^{\omega}(X_n)\big)^2\Big] \le \sum_{n\in\Lambda_L} \mathbb{E}^{\omega}(X_n^2) \end{aligned}$$

$$= \sum_{n\in\Lambda_L} \mathbb{E}^\omega(X_n) \qquad (\text{since } X_n^2 = X_n)$$
$$= \mathbb{E}^\omega\big(N^\omega_{-,L}(E)\big) \qquad (\text{using (3.26)}).$$

Using the above estimate in (3.29), we get

$$\sum_{L=1}^\infty \mathbb{P}\left(\omega : \frac{\big|N^\omega_{-,L}(E) - \mathbb{E}^\omega\big(N^\omega_{-,L}(E)\big)\big|}{\beta_L} > \eta\right) \leq \frac{1}{\eta^2}\sum_{L=1}^\infty \frac{1}{\beta_L^2}\mathbb{E}^\omega\big(N^\omega_{-,L}(E)\big) \tag{3.30}$$
$$= \frac{1}{\eta^2}\sum_{L=1}^\infty \frac{1}{\beta_L}\frac{1}{\beta_L}\mathbb{E}^\omega\big(N^\omega_{-,L}(E)\big)$$
$$\leq \frac{C}{\eta^2}\sum_{L=1}^\infty \frac{1}{\beta_L} \qquad (\text{using (3.10)})$$
$$\lesssim \sum_{L=1}^\infty \frac{1}{L^{d-\alpha(\delta-1)}} \qquad (\text{using (1.5)}).$$

As we have assumed in the theorem that $0 < \alpha < \frac{1}{2}$, $1 < \delta < \frac{1}{2\alpha}$ and $d \geq 2$, we have $d - \alpha(\delta - 1) > 1$. Thus, (3.28) follows from (3.30).

Therefore, from (3.27), for a.e. ω, we have

$$\lim_{L\to\infty} \frac{1}{\beta_L} N^\omega_{-,L}(E) = \lim_{L\to\infty} \frac{1}{\beta_L}\mathbb{E}^\omega\big(N^\omega_{-,L}(E)\big) \tag{3.31}$$
$$= \frac{1}{2\ \epsilon^{(\delta-1)}} \ (\text{using (3.10)}) = \frac{1}{2\ (-2d-E)^{(\delta-1)}} \ (E = -2d - \epsilon).$$

A similar calculation gives, for a.e. ω,

$$\lim_{L\to\infty} \frac{1}{\beta_L} N^\omega_{+,L}(E) = \lim_{L\to\infty} \frac{1}{\beta_L}\mathbb{E}^\omega\big(N^\omega_{+,L}(E)\big) \tag{3.32}$$
$$= \frac{1}{2\ (4d+\epsilon)^{(\delta-1)}} \ (\text{using (3.11)}) = \frac{1}{2\ (2d-E)^{(\delta-1)}} \ (E = -2d - \epsilon).$$

The inequalities (3.31), (3.32) together with (3.2) give, for $E < -2d$ for a.e. ω,

$$\frac{1}{2}\frac{1}{(2d-E)^{(\delta-1)}} \leq \varliminf_{L\to\infty} \frac{1}{\beta_L} N^\omega_L(E) \leq \varlimsup_{L\to\infty} \frac{1}{\beta_L} N^\omega_L(E) \leq \frac{1}{2}\frac{1}{(-2d-E)^{(\delta-1)}}. \tag{3.33}$$

For $E > 2d$ we compute $\tilde{N}^\omega_{\pm,L}(E)$ (as in (3.13)) exactly in the same way as given above. Thus, we can prove that, for a.e. ω,

$$\lim_{L\to\infty} \frac{1}{\beta_L} \tilde{N}^\omega_{+,L}(E) = \lim_{L\to\infty} \frac{1}{\beta_L}\mathbb{E}^\omega\big(\tilde{N}^\omega_{+,L}(E)\big) = \frac{1}{2\ (E-2d)^{(\delta-1)}}$$

and

$$\lim_{L\to\infty} \frac{1}{\beta_L} \tilde{N}^\omega_{-,L}(E) = \lim_{L\to\infty} \frac{1}{\beta_L}\mathbb{E}^\omega\big(\tilde{N}^\omega_{-,L}(E)\big) = \frac{1}{2\ (2d+E)^{(\delta-1)}}.$$

These equalities, together with (3.14) give the following. For $E > 2d$, a.e. ω,

$$\frac{1}{2}\frac{1}{(2d+E)^{(\delta-1)}} \leq \varliminf_{L\to\infty} \frac{1}{\beta_L}\tilde{N}_L^{\omega}(E) \leq \varlimsup_{L\to\infty} \frac{1}{\beta_L}\tilde{N}_L^{\omega}(E) \leq \frac{1}{2}\frac{1}{(E-2d)^{(\delta-1)}}. \quad (3.34)$$

□

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Boundary Values of Resolvents of Self-adjoint Operators in Krein Spaces and Applications to the Klein–Gordon Equation

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Abstract. The aim of this talk is to describe a generalization of the classical Mourre theorem [M1] to the Krein space setting. Applications to the Klein–Gordon equation are given. The talk is based on joint work with Vladimir Georgescu and Christian Gérard. Details of the proofs can be found in [GGH1] and [GGH2].

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1. Introduction

Let us consider on $\mathbb{R}^d$ the Klein–Gordon equation minimally coupled to an electric field.

$$(\partial_t - \mathrm{i}v(x))^2\phi(t,x) - \Delta_x\phi(t,x) + m^2\phi(t,x) = 0. \tag{1.1}$$

Here $v \in C^\infty(\mathbb{R}^d)$ is the electric potential and $m > 0$ the mass of the Klein–Gordon field. We consider the long-range case:

$$\exists\epsilon > 0,\ \forall\alpha \in \mathbb{N}^d,\ |\partial_x^\alpha v(x)| \lesssim \langle x\rangle^{-\epsilon-|\alpha|}.$$

The equation (1.1) admits a conserved energy:

$$\int_{\mathbb{R}^d} |\partial_t\phi(t,x)|^2 + |\nabla_x\phi(t,x)|^2 + (m^2 - v^2(x))|\phi(t,x)|^2\,dx.$$

Let us now write this equation as a first-order equation:

$$f(t) = \begin{pmatrix} \phi(t) \\ \mathrm{i}^{-1}\partial_t\phi(t) \end{pmatrix},\ f(t) = \mathrm{e}^{\mathrm{i}tH}f(0),\ H = \begin{pmatrix} 0 & \mathbb{1} \\ -\Delta_x + m^2 - v^2 & 2v \end{pmatrix}.$$

The energy then is written

$$E(f,f)=\int_{\mathbb{R}^d}|f_1|^2(x)+((-\Delta_x+m^2-v^2(x))f_0(x))\overline{f}_0(x)dx,\ f=\begin{pmatrix} f_0\\ f_1\end{pmatrix}.$$

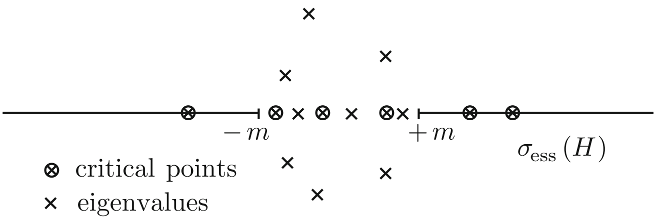
The problem consists in the fact that $h=-\Delta_x+m^2-v^2$ might acquire a *negative spectrum.* In this case the energy defines a non-degenerate quadratic form, but it is not positive. Such forms are usually called Krein forms and the corresponding spaces are called Krein spaces. The spectral theory for self-adjoint operators on Krein spaces was initiated by Bognar [B], Jonas [J1]–[J2] and Langer [La], and then pushed further by Langer–Najman–Tretter [LNT1]–[LNT2]. Scattering theory for the Klein–Gordon equation without positive energy was first developed by Kako [K] for short range potentials ($v(x)\in O(\langle x\rangle^{-2-\epsilon})$ and then by C. Gérard [Ge2] in the massive long-range case via time-dependent methods. The aim of this talk is to discuss scattering theory for self-adjoint operators on Krein spaces in a somewhat more general setting. In particular we will prove a generalization of the classical Mourre theorem to the Krein space setting. Before doing so, let us explain our results when applied to the concrete situation explained in this introduction. We define the energy space by

$$\mathcal{E}=H^1(\mathbb{R}^d)\oplus L^2(\mathbb{R}^d).$$

We then obtain

$$\sigma_{\text{ess}}(H)=]-\infty,-m]\cup[m,+\infty[$$
$$\sigma(H)\backslash\mathbb{R}=\cup_{1\le j\le n}\{\lambda_j,\overline{\lambda_j}\},$$

where λ_j, $\overline{\lambda_j}$ are eigenvalues of finite Riesz index.



For $s>1/2$ and some suitable $\delta>0$ we have:

$$\sup_{\mathrm{Re}z\in I,0<|\Im z|\le\delta}\|\langle x\rangle^{-s}(H-z)^{-1}\langle x\rangle^{-s}\|_{B(\mathcal{E})}<\infty,$$

where $I\subset\mathbb{R}$ is a compact interval disjoint from $\pm m$, containing no real eigenvalues of H, nor so-called *critical points* of H. We refer to Section 6.4 for more general results including the massless case.

We conclude this introduction with a comment on the situation on a cylindrical manifold $\mathbb{R}_x\times S^{d-1}_\omega$ when the potential has two different limits for $x\to\pm\infty$. This situation is very different in the sense that the Krein space setting can no longer be applied. According to the physics literature we speak in this situation loosely about super-radiance if h has negative spectrum. Examples are given by the charged Klein–Gordon field outside a Reissner–Nordström black hole or the wave equation outside a Kerr black hole. The first work concerning scattering theory for this problem in dimension 1 and for very short range potentials was published by Alain Bachelot in 2004 [Ba]. Similar results in dimension 3 have been obtained by V. Georgescu, C. Gérard and the author in [GGH3], applications to the De Sitter Kerr metric are given in this paper. However we won't discuss these issues in this talk.

1.1. Notations

If $\mathcal{H}$ is a Banach space we denote $\mathcal{H}^*$ its adjoint space, i.e., the set of continuous anti-linear functionals on $\mathcal{H}$ equipped with the natural Banach space structure. The canonical anti-duality between $\mathcal{H}$ and $\mathcal{H}^*$ is denoted $\langle u, w\rangle \equiv w(u)$, where $u \in \mathcal{H}$ and $w \in \mathcal{H}^*$. So $\langle \cdot, \cdot\rangle : \mathcal{H} \times \mathcal{H}^* \to \mathbb{C}$ is anti-linear in the first argument and linear in the second one. On the other hand, we denote by $\langle \cdot|\cdot\rangle$ hermitian forms on $\mathcal{H}$, again anti-linear in the first argument and linear in the second one.

We say that $\mathcal{H}$ is *Hilbertizable* if there is a scalar product on $\mathcal{H}$ such that the norm associated to it defines the topology of $\mathcal{H}$. Scalar products are denoted by $(\cdot|\cdot)$. If $\mathcal{H}$ is a reflexive Banach space then the canonical identification $\mathcal{H}^{**} = \mathcal{H}$ is obtained by setting $u(w) = \overline{w(u)}$ for $u \in \mathcal{H}$ and $w \in \mathcal{H}^*$. In other terms, the relation $\mathcal{H}^{**} = \mathcal{H}$ is determined by the rule $\langle w, u\rangle = \overline{\langle u, w\rangle}$.

Let $\mathcal{G}, \mathcal{H}$ be reflexive Banach spaces and $\mathcal{E} = \mathcal{G} \oplus \mathcal{H}$. The usual realization $(\mathcal{G} \oplus \mathcal{H})^* = \mathcal{G}^* \oplus \mathcal{H}^*$ of the adjoint space will not be convenient later, we shall rather identify $\mathcal{E}^* = \mathcal{H}^* \oplus \mathcal{G}^*$ in the obvious way.

If S is a closed densely defined operator on a Banach space $\mathcal{H}$, we denote by $\rho(S)$, $\sigma(S)$ its resolvent set and spectrum.

We use the notation $\langle a\rangle = (1 + a^2)^{\frac{1}{2}}$ if a is a real number or an operator for which this expression has a meaning.

2. Krein spaces

2.1. Basic definitions

We start with the basic definition of a Krein space:

Definition 1. A *Krein space* is a hilbertizable vector space $\mathcal{K}$ equipped with a *bounded hermitian sesquilinear* form $\langle \cdot|\cdot\rangle$ such that for any continuous linear form φ on $\mathcal{K}$ there is a unique $u \in \mathcal{K}$ such that $\varphi = \langle u|\cdot\rangle$. The form $\langle \cdot|\cdot\rangle$ is called the *Krein structure.*

Let $J : \mathcal{K} \to \mathcal{K}^*$ be the linear continuous map defined by $Ju = \langle \cdot|u\rangle$, so that $\langle u|v\rangle = \langle u, Jv\rangle$. J is bijective. Thus the Krein structure $\langle \cdot|\cdot\rangle$ allows us to identify $\mathcal{K}^*$ and $\mathcal{K}$ with the help of J.

We say that a linear subspace $\mathcal{H}$ is a *Hilbert subspace of* $\mathcal{K}$ if $\big(\mathcal{H}, \langle \cdot|\cdot\rangle|_{\mathcal{H}\times\mathcal{H}}\big)$ is a Hilbert space.

Proposition 1. *A Krein space is a reflexive Banach space.*

2.2. Operators on Krein spaces

2.2.1. Adjoints on Krein spaces. If $T \in B(\mathcal{K})$, then $T^* \in B(\mathcal{K}^*)$ is defined in the Banach space sense. We can transport it on $\mathcal{K}$ with the help of J. We then define the natural involution $T \mapsto T^*$ on $B(\mathcal{K})$ such that $\langle T^* u|v\rangle = \langle u|Tv\rangle$. This definition extends to closed densely defined operators. We say that an operator S is self-adjoint if $S^* = S$ and that an operator S is positive if $\langle u|Su\rangle \geq 0$ for all $u \in D(S)$.

2.2.2. Projections on Krein spaces. A projection on $\mathcal{K}$ is an element $\Pi \in B(\mathcal{K})$ such that $\Pi^2 = \Pi$. A self-adjoint projection is also called an orthogonal projection. A positive projection is a projection Π such that $\Pi \geq 0$. We have the useful proposition due to Bognar [B]

Proposition 2. *The range of a positive projection is a Hilbert subspace of $\mathcal{K}$. Reciprocally, if $\mathcal{H}$ is a Hilbert subspace of $\mathcal{K}$ then there is a unique self-adjoint projection Π such that $\Pi\mathcal{K} = \mathcal{H}$ and this projection is positive.*

3. Functional calculus

3.1. Smooth and Borel functional calculus on Banach spaces

Let $\mathcal{K}$ be a Banach space, H be a closed densely defined operator on $\mathcal{K}$ and $R(z)$ its resolvent.

Definition 2. Let $\beta(H)$ be the set of $\lambda \in \mathbb{R}$ such that there is a real open neighborhood I of λ and there are numbers $\nu > 0, n \in \mathbb{N}, C > 0$ such that $\|R(z)\| \leq C|\mathrm{Im} z|^{1-n}$ if $\mathrm{Re} z \in I$, $0 < |\mathrm{Im} z| \leq \nu$.

If $I \subset \beta(H)$ is an open interval and $\chi \in C_0^\infty(I)$, then we can define $\chi(H)$ by the Helffer–Sjöstrand formula:

$$\chi(H) = -\frac{1}{2\pi \mathrm{i}} \int_{\mathbb{C}} R(z)\overline{\partial}\tilde{\chi}(z) dz \wedge d\overline{z}.$$

We shall say that the smooth functional calculus extends to a C^0- functional calculus on I if $\|\chi(H)\| \leq C \sup_{\lambda\in I} |\chi(\lambda)|$ for all $\chi \in C_0^\infty(I)$. We then obtain a unique continuous extension to an algebra morphism $C_0(I) \to B(\mathcal{K})$. The proof is a straightforward application of the Riesz theorem, see, e.g., [Wr, Corollary 9.1.2].

Theorem 3.1. *Assume that $\mathcal{K}$ is a reflexive Banach space and let $F_0 : C_0(I) \to B(\mathcal{K})$ be a norm continuous algebra morphism. Then there is a unique algebra morphism $F : \mathcal{B}(I) \to B(\mathcal{K})$ which extends F_0 and such that:* b-$\lim_n \varphi_n = \varphi \Rightarrow F(\varphi_n) \to F(\varphi)$ *weakly.*

Here $\mathcal{B}(I)$ denotes the set of bounded Borel functions on I and b-$\lim_n \varphi_n = \varphi$ means that

$$\sup_{\lambda\in I,\, n\in\mathbb{N}} |\varphi_n(\lambda)| < \infty, \quad \lim \varphi_n(\lambda) = \varphi(\lambda),\ \forall \lambda \in I.$$

In this case we say that φ_n *converges boundedly* to φ on I.

3.2. C^0-groups

Let $W_t = \mathrm{e}^{itA}$ be a C_0-group on a Banach space $\mathcal{K}$ with generator A. Then there are numbers $M \geq 1$ and $\gamma \geq 0$ such that

$$\|W_t\| \leq M\mathrm{e}^{\gamma|t|} \quad \text{for all} \;\; t \in \mathbb{R}.$$

The spectrum of the operator A is then included in the strip $|\mathrm{Im}z| \leq \gamma$ and it could be equal to this strip. We say that $S \in B(\mathcal{K})$ is of class $C^\alpha(A)$ if the map

$$\mathbb{R} \ni t \mapsto S(t) = e^{-\mathrm{i}tA} S e^{\mathrm{i}tA} \in B(\mathcal{K})$$

is C^α for the strong operator topology. For an unbounded operator S we say that $S \in C^\alpha(A)$ if $R(z_0) = (S - z_0)^{-1} \in C^\alpha(A)$ for some $z_0 \in \rho(S)$. If $\mathcal{K}$ is a Krein space we say that the Krein structure is of class $C^1(A)$ if the conditions in the next proposition are verified.

Proposition 3. *The following assertions are equivalent:*

1. *the function $t \mapsto \langle W_t u | W_t u \rangle$ is derivable at zero for each $u \in \mathcal{H}$;*
2. *the function $t \mapsto \langle W_t u | W_t u \rangle$ is of class C^1 for each $u \in \mathcal{H}$;*
3. *the map $t \mapsto W_t^* W_t$ is locally Lipschitz;*
4. *$A^* = A + B$ where B is a bounded operator.*

3.3. $\mathcal{M}_\gamma$ functional calculus

Let $\mathcal{M}_\gamma$ be the set of functions $f : \mathbb{R} \to \mathbb{C}$ whose Fourier transforms are complex measures such that:

$$\|f\|_{\mathcal{M}_\gamma} := \int \mathrm{e}^{\gamma|t|} |\widehat{f}(t)| dt < \infty.$$

$\mathcal{M}_\gamma$ is a unital Banach $*$-algebra for the usual operations of addition and multiplication and $f^*(\tau) = \overline{f}(-\tau)$ as involution. If

$$\|W_t\| \leq M\mathrm{e}^{\gamma|t|}, \;\; t \in \mathbb{R},$$

then it follows that we can define $f(A)$ for $f \in \mathcal{M}_\gamma$ by the formula

$$f(A) = \int W_t \widehat{f}(t) dt.$$

$\mathcal{M}_\gamma \ni f \mapsto f(A) \in B(\mathcal{H})$ is a linear multiplicative map such that

$$\|f(A)\| \leq M_\gamma \|f\|_{\mathcal{M}_\gamma}.$$

We have for $\sigma > 0$, $\langle . \rangle^{-\sigma} \in \mathcal{M}_\gamma$ if $\gamma < 1/2$.

4. Boundary value estimates

4.1. Main theorem

Theorem 4.1. *Let $\mathcal{K}$ be a Krein space and A the generator of a C_0-group of operators on $\mathcal{K}$ such that the Krein structure is of class $C^1(A)$. Let H be a self-adjoint operator on $\mathcal{K}$ and Π a positive projection which commutes with H such that the following conditions are satisfied:*

1. *H is of class $C^\alpha(A)$ for some $\alpha > 3/2$, in particular $H' = [H, \mathrm{i}A]$ is well defined;*
2. *there is $\varphi \in C_0^\infty(\beta(H))$ real with $\varphi(\lambda) = 1$ on a neighborhood of a compact interval J such that $\varphi(H)\Pi = \varphi(H)$ and*

$$\varphi(H)(\mathrm{Re}H')\varphi(H) \geq a\varphi(H)^2,\ a > 0. \tag{4.2}$$

Then if $s > 1/2$ and $\varepsilon > 0$ is small enough, we have

$$\sup_{z \in J \pm \mathrm{i}]0,\nu]} \|\langle \varepsilon A\rangle^{-s} R(z) \langle \varepsilon A\rangle^{-s}\| < \infty, \text{ for some } \nu > 0.$$

Remark 1.

1. The above theorem is a generalization of the classical Mourre theorem to the Krein space setting. The condition $\alpha > 3/2$ is the condition which comes out naturally in the proof, but it is certainly not optimal.
2. In applications one often assumes that H admits a Borel functional calculus on an interval $I \supset J$ and that $\Pi = \mathbb{1}_I(H)$. If $\mathbb{1}_I(H) \leq 0$, then the assumption (4.2) should be replaced by

$$\varphi(H)(\mathrm{Re}H')\varphi(H) \leq a\varphi(H)^2,\ a > 0. \tag{4.3}$$

   To see this we replace the Krein form $\langle \cdot | \cdot \rangle$ by the Krein form $-\langle \cdot | \cdot \rangle$. With respect to this new Krein form we have $\mathbb{1}_I(H) \geq 0$ and (4.3) implies (4.2) for the new Krein form.

4.2. Virial theorem

In order to be able to apply the above theorem in concrete situations we need an equivalent of the virial theorem in the Krein space setting. We assume that H admits a Borel functional calculus on I, that $\lambda \in I$ and that $H \in C^1(A)$.

Lemma 1 (Virial Theorem). *For any $\lambda \in I$ we have:*

$$\mathbf{1}_{\{\lambda\}}(H)[iH, A]\mathbf{1}_{\{\lambda\}}(H) = 0.$$

Corollary 1. *Assume that for some $J \subset I$ we have $\mathbb{1}_J(H) \geq 0$ and that there is a number $a > 0$ and a compact operator K such that $\mathbb{1}_J(H)(ReH')\mathbb{1}_J(H) \geq a\mathbb{1}_J(H) + K$. Then the point spectrum of H in J is finite and consists of eigenvalues of finite multiplicity. Moreover, if $\lambda \in J$ is not an eigenvalue of H and $b < a$ then there is a compact neighborhood $\widehat{J}$ of λ in J such that $\mathbb{1}_{\widehat{J}}(H)(ReH')\mathbb{1}_{\widehat{J}}(H) \geq b\mathbb{1}_{\widehat{J}}(H)$.*

4.3. An important proposition

Proposition 4. *Let H be a self-adjoint operator with $\sigma(H) \neq \mathbb{C}$ on the Krein space $\mathcal{K}$. Let Π be a positive projection which commutes with H and let B, C, D be bounded operators such that*

(1) *$B = B^*$, $C = \Pi C$,*
(2) *$BC = CD$,*
(3) *$CC^* \leq \Pi[H, \mathrm{i}B]\Pi$ as quadratic forms on $D(H)$.*

Then the operator $L(z) = C^* R(z) C$ *satisfies*

$$\langle L(z)u | L(z)u \rangle \leq c(\|B\| + \|D\|)\|L(z)u\|\|u\| \quad \textit{for} \;\; u \in \mathcal{K}, \;\; z \notin \sigma(H),$$

where c *depends only on* $\mathcal{K}$ *and* Π.

The proof uses ideas of Putnam as well as of an earlier paper of C. Gérard [Ge1].

Proof. Let $\mathrm{Im} z \geq 0$. We have for $b \in \mathbb{R}$:

$$\begin{aligned} &R^*[H, \mathrm{i}B]R \\ &\quad = R^*[H - z, \mathrm{i}(B + b)]R = \mathrm{i}(B + b)R - R^* i(B + b) + (2\mathrm{Imz})\mathrm{R}^*(\mathrm{B} + \mathrm{b})\mathrm{R} \\ &\quad = 2\mathrm{Im}\big(R^*(B + b)\big) + (2\mathrm{Im} z) R^*(B + b)R. \end{aligned}$$

Since $(B + b)C = C(D + b)$ we get

$$C^* R^*[H, \mathrm{i}B]RC = 2\mathrm{Im}\big(C^* R^* C(D + b)\big) + (2\mathrm{Im} z) C^* R^*(B + b)RC. \tag{4.4}$$

Since $C = \Pi C$ and Π commutes with H we have

$$C^* R^*(B + b)RC = C^* R^* \Pi (B + b) \Pi RC.$$

Using $\pm \langle \Pi u | S \Pi u \rangle \leq \|S\|_{\Pi\mathcal{K}} \langle \Pi u | \Pi u \rangle$ we may choose $b = -\|B\|_{\Pi\mathcal{K}}$ such that $(2\mathrm{Im} z) C^* R^*(B + b)RC \leq 0$, hence from (4.4) we get:

$$C^* R^*[H, \mathrm{i}B]RC \leq 2\mathrm{Im}\big(L^*(D + b)\big).$$

Now observe that $C^* R^*[H, \mathrm{i}B]RC = C^* R^* \Pi [H, \mathrm{i}B] \Pi RC$ hence from hypothesis (3), we get

$$L^* L = C^* R^* C C^* RC \leq 2\mathrm{Im}\big(L^*(D + b)\big).$$

Now for $u \in \mathcal{K}$, with a constant m depending only on $\mathcal{K}$:

$$\langle Lu | Lu \rangle \leq 2\mathrm{Im} \langle Lu | (D + b)u \rangle \leq m\|Lu\|\|(D + b)u\| \leq m\|Lu\|(\|D\| + \|B\|_{\Pi\mathcal{K}})\|u\|,$$

using that $b = -\|B\|_{\Pi\mathcal{K}}$. Since $\|B\|_{\Pi\mathcal{K}} \leq d\|B\|$, for some constant d depending only on Π, this gives the required estimate for $c = \max(m, md)$. □

4.4. Idea of the proof of Theorem 4.1

Let I be an open neighborhood of J on which $\varphi(\lambda) = 1$. We notice that it suffices to show

$$\sup_{z \notin \mathbb{R}} \|\langle \varepsilon A \rangle^{-s} R(z) \xi(H)^2 \langle \varepsilon A \rangle^{-s}\| < \infty$$

for each real $\xi \in C_0^\infty(I)$. In the following $\xi = \xi(H)$. Let $g(\tau) = \langle \tau \rangle^{-s}$, f such that $f' = g^2$, and $g_\varepsilon = g(\varepsilon A), f_\varepsilon = f(\varepsilon A)$. Fix $\phi \in C_0^\infty(\mathbb{R})$ real such that $\phi(\lambda) = \lambda$ in a neighborhood of the support of φ and set $S = \phi(H)$. Let $F_\varepsilon := \varepsilon^{-1}\mathrm{Re} f_\varepsilon$. Then we have for ε small enough

$$[S, \mathrm{i}\xi F_\varepsilon \xi] \sim g_\varepsilon \xi (ReH') \xi g_\varepsilon^* \geq \frac{a}{2} \xi g_\varepsilon g_\varepsilon^* \xi.$$

Here $\sim$ is an equality modulo small error terms when ε goes to zero. We now apply the preceding Proposition with $B = \xi F_\varepsilon \xi$, $C = \xi g_\varepsilon$ and $D = g_\varepsilon^{-1} F_\varepsilon \xi^2 g_\varepsilon$. For $L_\epsilon = g_\epsilon^* \xi^2 R g_\epsilon$ we obtain:

$$\langle L_\varepsilon u | L_\varepsilon u \rangle \le K(\|B_\varepsilon\| + \|D_\varepsilon\|)\|L_\varepsilon u\|\|u\| \le \delta \|L_\varepsilon u\|^2 + (4\delta)^{-1}(\|B_\varepsilon\| + \|D_\varepsilon\|)^2 \|u\|^2.$$

Let $\eta \in C_0^\infty(I)$ such that $\eta\xi = \xi$. We have $\Pi\eta = \eta$, $N^{-1}\|v\|^2 \le \langle v|v\rangle$ for $v \in \Pi\mathcal{K}$ and

$$(1-\eta)L_\epsilon = [g_\varepsilon^*, \eta]\xi^2 R g_\epsilon = O(\epsilon) L_\epsilon.$$

5. Definitizable operators on Krein spaces

5.1. Definitizable operators

Definition 3. A self-adjoint operator H is *definitizable* if $\rho(H) \ne \emptyset$ and there exists a real polynomial $p \ne 0$ such that $\langle u | p(H) u\rangle \ge 0,\ \forall\ u \in \mathrm{Dom} H^k,\ k := \deg p$. H is said to be even definitizable if k can be chosen to be even.

Remark 2. $p(z)$ in Definition 3 can be replaced by ($z_0 \in \rho(H)$):

$$q(z) = \frac{p(z)}{(z - z_0)^k (z - \overline{z_0})^k}, \quad \begin{array}{ll} k = \deg p/2 & \text{if } \deg p \text{ even}, \\ k = (\deg p + 1)/2 & \text{if } \deg p \text{ odd}. \end{array}$$

If λ is an isolated point of $\sigma(H)$ we define the Riesz spectral projection

$$E(\lambda, H) := \frac{1}{2\mathrm{i}\pi} \oint_C (z - H)^{-1} dz,$$

where C is a small curve in $\rho(H)$ surrounding λ. For the proof of the following Proposition see [J1, Lemma 1]

Proposition 5. *Let H be a definitizable self-adjoint operator. Then:*

1. *If $z \in \sigma(H)\backslash\mathbb{R}$ then $p(z) = 0$ for each definitizing polynomial p.*
2. *There is a definitizing polynomial p such that $\sigma(H) \setminus \mathbb{R}$ is exactly the set of non-real zeroes of p.*
3. *$\sigma(H)\backslash\mathbb{R}$ is a finite union of pairs $\{\lambda_i, \overline{\lambda_i}\}$ of eigenvalues of finite Riesz index.*

We set now

$$\mathbb{1}_{\mathrm{pp}}^{\mathbb{C}} = \sum_{\lambda \in \sigma(H),\ \mathrm{Im}\lambda > 0} E(\lambda, H) + E(\overline{\lambda}, H),\ \mathcal{K}_{\mathrm{pp}}^{\mathbb{C}} := \mathbb{1}_{\mathrm{pp}}^{\mathbb{C}} \mathcal{K}.$$

Then $\mathbb{1}_{\mathrm{pp}}^{\mathbb{C}}$ is a projection, $\mathbb{1}_{\mathrm{pp}}^{\mathbb{C}} = (\mathbb{1}_{\mathrm{pp}}^{\mathbb{C}})^*$, hence $\mathcal{K}_{\mathrm{pp}}^{\mathbb{C}}$ is a Krein space and

$$\mathcal{K} = \mathcal{K}_{\mathrm{pp}}^{\mathbb{C}} \oplus (\mathcal{K}_{\mathrm{pp}}^{\mathbb{C}})^\perp =: \mathcal{K}_{\mathrm{pp}}^{\mathbb{C}} \oplus \mathcal{K}_1.$$

Remark 3. Because of the above splitting, we have $H = H_1 \oplus H_2$, where $H_1 = H|_{\mathcal{K}_{\mathrm{pp}}^{\mathbb{C}}}$ and $H_2 = H|_{\mathcal{K}_1}$. For every "reasonable" function ϕ we should have $\phi(H) = \phi(H_1) \oplus \phi(H_2)$. The definition of $\phi(H_1)$ being rather obvious, it is enough to suppose $\sigma(H) \subset \mathbb{R}$ when we discussing functional calculus for definitizable operators.

Definition 4. Let H, p as above. Set $c_p(H) := p^{-1}(\{0\}) \cap \sigma(H) \cap \mathbb{R}$.

1. The set $c_{\text{fin}}(H)$ equal to the intersection of the $c_p(H)$ for all definitizing polynomials for H is called the set of (*finite*) *critical points* of H.
2. The set $c(H) := c_{\text{fin}}(H) \cup \{\infty\}$ considered as a subset of the one-point compactification $\hat{\mathbb{C}} := \mathbb{C} \cup \{\infty\}$ is called the set of *critical points* of H.

Definition 5. Let H be a definitizable operator on $\mathcal{K}$. For $\lambda_j \in c_{\text{fin}}(H)$ we denote by k_j the minimum over all definitizing polynomials p with $p(\lambda_j) = 0$, of the multiplicity of λ_j as a zero of p. For $\lambda = \infty$, we set $\kappa = 0$ if H is even definitizable and $\kappa = 1$ otherwise. We denote by $\mathcal{C}(H)$ the set

$$\mathcal{C}(H) = \{(\lambda_j, k_j)\} \cup \{(\infty, \kappa)\},$$

obtained with these conventions.

Definition 6. Let $k \in \mathbb{N}$ and $f : \mathbb{R} \to \mathbb{C}$.

1. we say that f is of class C^k at $\lambda \in \mathbb{R}$ if there is a polynomial p with $\deg p \leq k$ such that: $f(x) = p(x) + o((x-\lambda)^k)$;
2. we say that f is of class C^0 at $\lambda = \infty$ if f is bounded in a neighborhood of $\pm\infty$ in $\mathbb{R}$.
3. we say that f is of class C^1 at $\lambda = \infty$ if there exists a constant f_∞ such that $f(x) = f_\infty + o(x^{-1})$ near $\pm\infty$.

For $l \leq k$ we denote by $p_l(x)$ the part of p of degree less or equal $l-1$ so that $f(x) - p_l(x) \in 0((x-\lambda)^l)$.

Definition 7. We denote by $\mathcal{B}_{\mathcal{C}(H)}(\mathbb{R})$ the $*$-algebra of bounded Borel functions f on $\mathbb{R}$ such that f is of class C^{k_j} at each λ_j and of class C^κ at ∞. We equip $\mathcal{B}_{\mathcal{C}(H)}(\mathbb{R})$ with the norm:

$$\|f\|_{\mathcal{C}(H)} := \sup_{x\in\mathbb{R}} |f(x)| + \sum_{(\lambda_j,k_j)\in\mathcal{C}(H)} \sum_{0\leq l\leq k_j} \sup_{x\in\mathbb{R}} \left| \frac{f(x)-p_l(x)}{(x-\lambda_j)^l} \right| + \sup_{|x|\geq 1} \kappa \left| x(f(x)-f_\infty) \right|.$$

Let H be a definitizable operator with $\sigma(H) \subset \mathbb{R}$ and $\mathcal{R}$ be the set of bounded rational functions $\varphi : \mathbb{R} \to \mathbb{C}$. We can easily define a *rational functional calculus* $\varphi(H)$, $\varphi \in \mathcal{R}$. For this functional calculus we obtain the estimate

$$\|\varphi(H)\| \leq C\|\varphi\|_{\mathcal{C}(H)}, \forall \varphi \in \mathcal{R}. \tag{5.5}$$

It thus extends to $\mathcal{B}_{\mathcal{C}(H)}(\mathbb{R})$:

Theorem 5.1. *Let H be a self-adjoint definitizable operator on the Krein space $\mathcal{K}$ with $\sigma(H) \subset \mathbb{R}$.Then there is a unique linear continuous map $\varphi \mapsto \varphi(H)$ from $\mathcal{B}_{\mathcal{C}(H)}(\mathbb{R})$ into $B(\mathcal{K})$ with the two following properties*

1. *if $\varphi(\lambda) = (\lambda - z)^{-1}$ for some non-real z, then $\varphi(H) = (H-z)^{-1}$,*
2. *if $\mathrm{b-}\lim_n \varphi_n = \varphi$ for $\varphi_n \in \mathcal{B}_{\mathcal{C}(H)}(\mathbb{R})$, then $\varphi(H) = \mathrm{w-}\lim \varphi_n(H)$.*

This map is a morphism of unital $*$-algebras.

Corollary 2. *If H is in addition even definitizable, then it is the generator of a unitary C_0-group on $\mathcal{K}$.*

Lemma 2. *Let $I \subset \mathbb{R}$ a bounded interval such that there exists a definitizing polynomial p with $\pm p(x) > 0$ for $x \in I$. Then*

$$\pm\langle u|\mathbb{1}_I(H)u\rangle \geq 0, \ u \in \mathcal{K}.$$

Let H be a definitizable operator. Let σ_c be the set of all complex eigenvalues of H. If $\lambda_j \in \sigma_c$ is a complex eigenvalue of H we define k_j as the order of the pole of $(H-z)^{-1}$. We denote $\mathcal{C}^{\mathbb{C}}(H)$ the set

$$\mathcal{C}^{\mathbb{C}}(H) = \{(\lambda_j, k_j)\}$$

obtained with these conventions.

Proposition 6. *We have*

$$\begin{aligned}\|(H-z)^{-1}\| \lesssim & \sum_{(\lambda_j,k_j)\in\mathcal{C}^{\mathbb{C}}} |z-\lambda_j|^{-k_j} \\ & + |\mathrm{Im} z|^{-1}\left(1 + \sum_{(\lambda_j,k_j)\in\mathcal{C}\setminus\{(\infty,\kappa)\}} |z-\lambda_j|^{-k_j} + |z|^{\kappa}\right)\end{aligned}$$

for all $z \notin \sigma_c \cup \mathbb{R}$.

To prove the proposition we apply the estimate (5.5) to $\varphi(x) = (x-z)^{-1}$.

5.2. Pontryagin spaces

Let $\mathcal{K}$ be a Krein space. We fix a scalar product $(\cdot|\cdot)$ on $\mathcal{K}$ endowing $\mathcal{K}$ with its hilbertizable topology. By the Riesz theorem we know that

$$\langle u|v\rangle = (u|Mv), \ u, v \in \mathcal{K},$$

where M is a bounded, invertible and self-adjoint operator. By the polar decomposition of M, we can write $M = J|M|$ where $J = J^*$, $J^2 = \mathbb{1}$. We can therefore introduce an equivalent scalar product:

$$(u|v)_M := (u||M|v),$$

so that

$$\langle u|v\rangle = (u|Jv)_M, \ u, v \in \mathcal{K}.$$

Definition 8. A Krein space $(\mathcal{K}, \langle\cdot|\cdot\rangle)$ is a *Pontryagin space* if either $\mathbb{1}_{\mathbb{R}^-}(J)$ or $\mathbb{1}_{\mathbb{R}^+}(J)$ has finite rank.

We have the following useful theorem (see [La]):

Theorem 5.2. *A self-adjoint operator H on a Pontryagin space is definitizable with an even definitizing polynomial p.*

6. Abstract Klein–Gordon equation

In this section we will apply our results to an abstract Klein–Gordon equation.

6.1. Energy spaces

We consider

$$\partial_t^2\phi(t) - 2\mathrm{i}k\partial_t\phi(t) + h\phi(t) = 0,$$

where $\phi : \mathbb{R} \to \mathcal{H}$, $\mathcal{H}$ is a (complex) Hilbert space, $h \in B(\mathcal{H})$ self-adjoint, $k : \langle h\rangle^{-\frac{1}{2}}\mathcal{H} \to \mathcal{H}$ symmetric, bounded. There is a conserved energy for this equation which is written

$$\|\partial_t\phi\|^2 + (h\phi|\phi).$$

We introduce the non-homogeneous energy space $\mathcal{E}$:

$$\mathcal{E} := \langle h\rangle^{-\frac{1}{2}}\mathcal{H} \oplus \mathcal{H}.$$

Lemma 3.

1. *If* $0 \in \rho(h)$ *then* $\mathcal{E}$ *equipped with the hermitian sesquilinear form:*

$$(f|f)_\mathcal{E} := (f_0|hf_0) + (f_1|f_1)$$

is a Krein space.

2. *if in addition* $\mathrm{Tr}\mathbb{1}_{]-\infty,0]}(h) < \infty$, *then* $(\mathcal{E},\ (\cdot|\cdot)_\mathcal{E})$ *is Pontryagin.*

We also introduce the homogeneous energy space $\dot{\mathcal{E}}$. Assume that $\mathrm{Ker}\, h = \{0\}$. We put

$$\dot{\mathcal{E}} := |h|^{-\frac{1}{2}}\mathcal{H} \oplus \mathcal{H}.$$

We have $\mathcal{E} \subset \dot{\mathcal{E}}$ continuously and densely. We have $\mathcal{E} = \dot{\mathcal{E}}$ iff $0 \in \rho(h)$.

Lemma 4. *Assume that* $\mathrm{Ker} h = \{0\}$. *Then* $\dot{\mathcal{E}}$ *equipped with* $(\cdot|\cdot)_\mathcal{E}$ *is a Krein space. If in addition* $\mathrm{Tr}\mathbb{1}_{]-\infty,0]}(h) < \infty$, *then* $\dot{\mathcal{E}}$ *is Pontryagin.*

Remark 4 (Charge spaces). If we put

$$f(t) = \begin{pmatrix} \phi(t) \\ \mathrm{i}^{-1}\partial_t\phi(t) - k\phi(t) \end{pmatrix},$$

then the charge

$$q(f,f) = (f_1|f_0) + (f_0|f_1)$$

is conserved. If we put $\mathcal{K}_\theta = \langle h\rangle^{-\theta}\mathcal{H} \oplus \langle h\rangle^{\theta}\mathcal{H}$, $0 \le \theta \le 1/2$, then $(\mathcal{K}_\theta, q)$ is a Krein space. We have $\mathcal{K}_{1/4} = [\mathcal{E}, \mathcal{E}^*]_{1/2}$ (complex interpolation space) and analogous results to the results presented here hold on $\mathcal{K}_{1/4}$. $\mathcal{K}_{1/4}$ is usually called the non-homogeneous charge space.

6.2. Klein–Gordon operators

$$H := \dot{H} := \begin{pmatrix} 0 & 1\!\!1 \\ h & 2k \end{pmatrix},$$

$$D(H) := \langle h\rangle^{-1}\mathcal{H} \oplus \langle h\rangle^{-\frac{1}{2}}\mathcal{H},$$

$$D(\dot{H}) := \left(|h|^{-\frac{1}{2}}\mathcal{H} \cap |h|^{-1}\mathcal{H}\right) \oplus \langle h\rangle^{-\frac{1}{2}}\mathcal{H}.$$

We have $\mathcal{E} \subset \dot{\mathcal{E}}$ and $D(H) \subset D(\dot{H})$ continuously and densely. H may also be considered as an operator acting in $\dot{\mathcal{E}}$, $\dot{H}$ is its closure in $\dot{\mathcal{E}}$.

Theorem 6.1.

1. *Assume that* $0 \in \rho(h)$. *Then* H *is a self-adjoint operator on the Krein space* $(\mathcal{E}, (\cdot|\cdot)_{\mathcal{E}})$ *with* $\rho(H) \neq \emptyset$.
2. *If in addition* $\mathrm{Tr} 1\!\!1_{]-\infty,0]}(h) < \infty$, *then* H *is even-definitizable.*

   Let $p(z) = h + z(2k - z)$. We denote by $\rho(h,k)$ the set of $z \in \mathbb{C}$ such that

$$p(z) : \langle h\rangle^{-1/2}\mathcal{H} \tilde{\rightarrow} \langle h\rangle^{1/2}\mathcal{H}$$

is a homeomorphism.

Theorem 6.2.

1. *Assume that there exists* $z \in \rho(h,k)$, $z \neq 0$. *Then* $\dot{H}$ *is self-adjoint on* $(\dot{\mathcal{E}}, (\cdot|\cdot)_{\mathcal{E}})$ *with* $\rho(\dot{H}) \neq \emptyset$.
2. *If in addition* $\mathrm{Tr} 1\!\!1_{]-\infty,0]}(h) < \infty$, *then* $\dot{H}$ *is even-definitizable.*

6.3. Limiting absorption principle

We will introduce 3 sets of hypotheses.

1. Energy (E):

$$\text{(E1)}\ \mathrm{Ker}\, h = \{0\}, \quad \text{(E2)}\ Tr 1\!\!1_{]-\infty,0]}(h) < \infty, \quad \text{(E3)}\ k|h|^{-1/2} \in B(\mathcal{H}).$$

2. Asymptotics (A): $h = b^2 - r$ with

$$\begin{aligned} &\text{(A1)} \quad b \geq 0, \text{ self-adjoint on } \mathcal{H},\ b^2 \sim |h|, \\ &\text{(A2)} \quad r \text{ symmetric on } \langle h\rangle^{-\frac{1}{2}}\mathcal{H},\ b^{-1}rb^{-1} \in B(\mathcal{H}), \\ &\text{(A3)} \quad k\langle b\rangle^{-1},\ b^{-1}rb^{-1} \in B_\infty(\mathcal{H}). \end{aligned}$$

   Here $b^2 \sim |h|$ means that $D(b) = D(|h|^{1/2})$ and that there exists a positive constant $c > 0$ such that

$$c^{-1}b \leq |h|^{1/2} \leq cb \text{ on } D(b).$$

3. Conjugate operator (M): Let a be a self-adjoint operator on $\mathcal{H}$ such that

$$\text{(M1)} \quad b^2 \in C^2(a).$$

Then $a_\chi = \chi(b^2)a\chi(b^2)$ is essentially self-adjoint on $D(a)$. We still denote by a_χ its closure.

$$\text{(M2)} \quad k\langle b\rangle^{-1}, \langle b\rangle^{-1}rb^{-1} \in C^2(a_\chi;\mathcal{H}), b^{-1}rb^{-1} \in C^1(a_\chi;\mathcal{H}),$$

$$\text{(M3)} \quad \begin{cases} \text{(i)} \quad \langle a_\chi\rangle\langle x\rangle^{-1} \in B(\mathcal{H}),\ \forall\, \chi \in C_0^\infty(\mathbb{R}), \\ \text{(ii)} \quad [\langle b\rangle, \langle x\rangle^{-\delta}]\langle x\rangle^{\delta} \in B(\mathcal{H}),\ 0 \le \delta \le 1. \end{cases}$$

Let $\tau(b^2)$ be the set of *thresholds* for (b^2, a): if $\lambda \notin \tau(b^2)$ there exists an interval $I \subset \mathbb{R}$, with $\lambda \in I$, a constant $c_0 > 0$ and $R \in B_\infty(\mathcal{H})$ such that

$$\mathbb{1}_I(b^2)[b^2, \mathrm{i}a]\mathbb{1}_I(b^2) \quad \ge \quad c_0\mathbb{1}_I(b^2) + R.$$

We also put

$$\tau(b) \quad := \quad \sqrt{\tau(b^2)}.$$

In the following we will write (E) for (E1)–(E3), (A) for (A1)–(A3) and (M) for (M1)–(M3).

Theorem 6.3. *Assume* (E), (A), (M). *Let* $I \subset \mathbb{R}^\pm$ *a compact interval such that*

$$\text{i) } I \cap \pm\tau(b) = \emptyset, \quad \text{ii) } I \cap c(\dot H) = \emptyset, \quad \text{iii) } 0 \notin I, \quad \text{iv) } \sigma_p(\dot H) \cap I = \emptyset.$$

We also suppose $\chi \in C_0^\infty(I)$. *Then there exists* $\epsilon_0 > 0$ *s. t. for* $\frac{1}{2} < \delta \le 1$*:*

$$\sup_{\mathrm{Re}z \in I,\ 0<|\mathrm{Im}z| \le \epsilon_0} \|(\langle x\rangle^{-\delta})_{\mathrm{diag}}(H-z)^{-1}(\langle x\rangle^{-\delta})_{\mathrm{diag}}\|_{B(\mathcal{E})} < \infty,$$

$$\int_{\mathbb{R}} \|(\langle x\rangle^{-\delta})_{\mathrm{diag}} \mathrm{e}^{\mathrm{i}tH}\chi(H)(\langle x\rangle^{-\delta})_{\mathrm{diag}}\varphi\|_{\mathcal{E}}^2 \lesssim \|\varphi\|^2.$$

Remark 5. We define the mass $m^2 = \inf(\sigma(h) \cap \mathbb{R}^+)$, $m \ge 0$. In the massless case $(m = 0)$, H admits a Borel functional calculus although $(\mathcal{E}, (.|.)_\mathcal{E})$ is not a Krein space.

6.4. Example: Charged Klein–Gordon equations on scattering manifolds

Let $\mathcal{N}$ be a smooth, $d-1$-dimensional compact manifold. Let $\mathcal{M}$ be a manifold of the form

$$\mathcal{M} \simeq \mathcal{M}_0 \cup\,]1, +\infty[_s \times \mathcal{N}_\omega,$$

where $\mathcal{M}_0 \Subset \mathcal{M}$ is relatively compact. For $m \in \mathbb{R}$ let $S^m(\mathcal{M})$ be the set of real-valued functions $f \in C^\infty(\mathcal{M})$ such that

$$\forall\, k \in \mathbb{N},\, \alpha \in \mathbb{N}^{d-1}, \quad |\partial_s^k \partial_\omega^\alpha f(s,\omega)| \le C_{k,\alpha}s^{m-k} \quad \text{for} \quad (s,\omega) \in]1,\infty[\times\mathcal{N}.$$

Definition 9. A Riemannian metric g^0 on $\mathcal{M}$ is called *conic* if there exists $R > 0$ and a Riemannian metric h on $\mathcal{N}$ such that

$$g^0 = ds^2 + s^2h_{jk}(\omega)d\omega^j d\omega^k \quad \text{for} \quad (s,\omega) \in [R,\infty[\times\mathcal{N}.$$

A Riemannian metric g on $\mathcal{M}$ is called a *scattering metric* if $g = g^0 + m$, where g^0 is a conic metric and m is of the form

$$m = m^0(s,\omega)ds^2 + sm_j^1(s,\omega)(dsd\omega^j + d\omega^j ds) + s^2m_{jk}^2(s,\omega)d\omega^j d\omega^k$$

with $m^l \in S^{-\mu_l}(\mathcal{M})$ for $l = 0, 1, 2$, $\mu_l > 0$.

Now the Klein–Gordon equation on $\mathcal{M}$ is written:

$$(\partial_t - \mathrm{i}v)^2\phi - (\nabla_k - \mathrm{i}A_k)(\nabla^k - \mathrm{i}A^k)\phi + m^2\phi = 0,$$

where ∇ is the Levi-Civita connection, v is the electric potential, $A_k(s,\omega)dx^k$ the magnetic potential and m the mass of the field.

After a unitary transformation the equation is written in local coordinates ($g = \det g$):

$$(\partial_t - \mathrm{i}v)^2\psi - g^{-1/4}(\partial_j - \mathrm{i}A_j)g^{1/2}g^{jk}(\partial_k - \mathrm{i}A_k)g^{-1/4}\psi + m^2(s,\omega)\psi = 0,$$

$\mathcal{H} = L^2(\mathcal{M}; dsd\omega)$, $p = -g^{-1/4}\partial_j g^{1/2}g^{jk}\partial_k g^{-1/4}$. Our assumptions are the following:

$$\begin{array}{l} A_j(s,\omega),\ m(s,\omega) - m_\infty \in S^{-\mu_0}(\mathcal{M}),\ \mu_0 > 0, \\ m_\infty := \lim_{s\to\infty} m(s,\omega) \geq 0. \end{array} \tag{6.6}$$

We assume that $v = v(s,\omega)$ is a multiplication operator and

$$\begin{aligned} &v(s,\omega) = v_\mathrm{l}(s,\omega) + v_\mathrm{s}(s,\omega),\ v_\mathrm{l}(s,\omega) \in S^{-\mu_0}(\mathcal{M}), \\ &v_\mathrm{s}(s,\omega)\langle p\rangle^{-1/2} \in B_\infty(\mathcal{H}),\ \langle s\rangle^2 v_\mathrm{s}(s,\omega)\langle p\rangle^{-1/2} \in B(\mathcal{H}). \end{aligned} \tag{6.7}$$

As a conjugate operator we use as usual the generator of dilations

$$a = \frac{1}{2}(\eta(s)sD_s + D_s s\eta(s)),$$

where $\eta \in C^\infty(\mathbb{R}, \mathbb{R}^+)$with $\eta(s) = 1$ for $s \geq 2$ and $\eta(s) = 0$ for $s \leq 1$.

Proposition 7 (Massive case). *Assume* (6.6), (6.7), $m_\infty > 0$ *and* $\operatorname{Ker} h = \{0\}$. *Then we have*

1. $\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ess}}(\dot{H}) =]-\infty, -m_\infty] \cup [m_\infty, +\infty[$;
2. *conditions* (E), (A), (M) *are satisfied;*
3. *one has* $\tau(b) = \{m_\infty\}$.

For the massless case we require instead of (6.7)

$$\begin{aligned} &v(s,\omega) = v_l(s,\omega) + v_s(s,\omega), \\ &\exists\ R_0 > 1,\ 0 \leq \delta < 1 \text{ such that } |v_l(s,\omega)| \leq \delta\tfrac{d-2}{2}\langle s\rangle^{-1},\ \text{for } s \geq R_0, \\ &sv_s\langle p\rangle^{-1/2} \in B_\infty(\mathcal{H}),\ s^3 v_s\langle p\rangle^{-1/2} \in B(\mathcal{H}). \end{aligned} \tag{6.8}$$

(6.8) permits us to use Hardy's inequality to deal with v_l.

Proposition 8 (Massless case). *Assume* (6.6) *with* $m_\infty = 0$, (6.8), $\operatorname{Ker} h = \{0\}$ *and* $d \geq 3$. *Then we have*

1. $\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ess}}(\dot{H}) = \mathbb{R}$;
2. *conditions* (E), (A), (M) *are satisfied;*
3. *one has* $\tau(b) = \{0\}$.

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Levinson's Theorem: An Index Theorem in Scattering Theory

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Abstract. A topological version of Levinson's theorem is presented. Its proof relies on a C^*-algebraic framework which is introduced in detail. Various scattering systems are considered in this framework, and more coherent explanations for corrections due to threshold effects or for a regularization procedure are provided. Potential scattering, point interactions, Friedrichs' model and Aharonov–Bohm's operators are some of the examples we have presented. Every concept that we have from scattering theory or from K-theory is introduced from scratch.

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1. Introduction

Levinson's theorem is a relation between the number of bound states of a quantum mechanical system and an expression related to the scattering part of that system. Its original formulation was established by N. Levinson in [35] in the context of a Schrödinger operator with a spherically symmetric potential, but subsequently numerous authors extended the validity of such a relation in various contexts or for various models. It is certainly impossible to quote all papers or books containing either Levinson's theorem in their title or in the subtitle of a section, but let us mention a few key references [6, 23, 36, 37, 38, 39, 40, 49, 45]. Various methods have also been used for the proof of this relation, as for example the Jost functions, the Green functions, the Sturm–Liouville theorem, and most prominently the spectral shift function. Note that expressions like the phase shift, the Friedel sum rule or some trace formulas are also associated with Levinon's theorem.

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Our aim in this review paper[1] is to present a radically different approach for Levinson's theorem. Indeed, during the last couple of years it has been shown that, once recast in a C^*-algebraic framework, this relation can be understood as an index theorem in scattering theory. This new approach does not only shed new light on this theorem, but also provides a more coherent and natural way to take various corrections or regularization processes into account. In brief, the key point in our proof of Levinson's theorem consists in evaluating the index of the wave operator by the winding number of an expression involving not only the scattering operator, but also new operators that describe the system at thresholds energies.

From this short description, it clearly appears that this new approach relies on two distinct fields of mathematics. On the one hand, the wave operators and the scattering operator belong to the framework of spectral and scattering theory, two rather well-known subjects in the mathematical physics community. On the other hand, the index theorem, winding numbers, and beyond them index maps, K-theory and Connes' pairing are familiar tools for operator algebraists. For this reason, special attention has been given to briefly introduce all concepts which belong only to one of these communities. One of our motivations in writing this survey is to make this approach of Levinson's theorem accessible to both readerships.

Let us now be more precise about the organization of this paper. In Section 2 we introduce a so-called "baby model" on which the essence of our approach can be fully presented. No prior knowledge on scattering theory or on K-theory is necessary, and all computations can be explicitly performed. The construction might look quite *ad hoc*, but this feeling will hopefully disappear once the full framework is established.

Section 3 contains a very short introduction to scattering theory, with the main requirements imposed on the subsequent scattering systems gathered in Assumption 3.1. In Section 4 we gradually introduce the C^*-algebraic framework, starting with a brief introduction to K-theory followed by the introduction of the index map. An abstract topological Levinson theorem is then proposed in Theorem 4.4. Since this statement still contains an implicit condition, we illustrate our purpose by introducing in Section 4.4 various isomorphic versions of the algebra which is going to play a key role in subsequent examples. In the last part of this section we show how the previous computations performed on the baby model can be explained in this algebraic framework. Clearly, Sections 3 and 4 can be skipped by experts in these respective fields, or very rapidly consulted for notations.

In Section 5 we gather several examples of scattering systems which are either one-dimensional or essentially one-dimensional. With the word "essential" we mean that a rather simple reduction of the system under consideration leads to a system which is not trivial only in a space of dimension one. Potential scattering on $\mathbb{R}$ is

[1]This paper is an extended version of a mini-course given at the *International conference on spectral theory and mathematical physics* which took place in Santiago (Chile) in November 2014. The author takes this opportunity to thank the organizers of the conference for their kind invitation and support.

presented and an explanation of the usual $\frac{1}{2}$-correction is provided. With another example, we show that embedded or non-embedded eigenvalues play exactly the same role for Levinson's theorem, a question which had led to some controversies in the past [15]. A sketchy presentation of a few other models is also proposed, and references to the corresponding papers are provided.

With Section 6 we start the most analytical section of this review paper. Indeed, a key role in our approach is played by the wave operators, and a good understanding of them is thus necessary. Prior to our investigations such a knowledge of these operators was not available in the literature, and part of our work has consisted in deriving new explicit formulas for these operators. In the previous section the resulting formulas are presented but not their proofs. In Section 6.1 we provide a rather detailed derivation of these formulas for a system of potential scattering in $\mathbb{R}^3$, and the corresponding computations are based on a stationary approach of scattering theory. On the algebraic side this model is also richer than the ones contained in Section 5 in the sense that a slight extension of the algebraic framework introduced in Section 4 together with a regularization procedure are necessary. More precisely, we provide a regularized formula for the computation of the winding number of suitable elements of $C\big(\mathbb{S};\mathcal{K}_p(\mathfrak{h})\big)$, the algebra of continuous functions on the unit circle with value in the pth Schatten class of a Hilbert space $\mathfrak{h}$.

A very brief description of wave operators for potential scattering in $\mathbb{R}^2$ is provided in Section 7. However, note that for this model a full understanding of wave operators is not available yet, and that further investigations are necessary when resonances or eigenvalues take place at the threshold energy 0. Accordingly, a full description of a topological Levinson theorem does not exist yet.

In Section 8 we extend the C^*-algebraic framework in a different direction, namely to index theorems for families. First of all, we introduce a rather large family of self-adjoint operators corresponding to the so-called Aharonov–Bohm operators. These operators are obtained as self-adjoint extensions of a closed operator with deficiency indices $(2,2)$. A Levinson theorem is then provided for each of them, once suitably compared with the usual Laplace operator on $\mathbb{R}^2$. For this model, explicit formulas for the wave operators and for the scattering operator are provided, and a thorough description of the computation of the winding number is also given. These expressions and computations are presented in Sections 8.1 and 8.2.

In order to present a Levinson theorem for families, additional information on cyclic cohomology, n-traces and Connes' pairing are necessary. A very brief survey is provided in Section 8.3. A glimpse on dual boundary maps is also given in Section 8.4. With this information at hand, we derive in Section 8.5 a so-called higher degree Levinson theorem. The resulting relation corresponds to the equality between the Chern number of a vector bundle given by the projections on the bound states of the Aharonov–Bohm operators, and a 3-trace applied to the scattering part of the system. Even if a physical interpretation of this equality is still lacking, it is likely that it can play a role in the theory of topological transport and/or adiabatic processes.

Let us now end this Introduction with some final comments. As illustrated by the multiplicity of the examples, the underlying C^*-algebraic framework for our approach of Levinson's theorem is very flexible and rich. Beside the extensions already presented in Sections 6 and 8, others are appealing. For example, it would certainly be interesting to recast the generalized Levinson theorem exhibited in [44, 55] in our framework. Another challenging extension would be to find out the suitable algebraic framework for dealing with scattering systems described in a two-Hilbert spaces setting. Finally, let us mention similar investigations [5, 53] which have been performed on discrete systems with the same C^*-algebraic framework in the background.

2. The baby model

In this section we introduce an example of a scattering system for which everything can be computed explicitly. It will allow us to describe more precisely the kind of results we are looking for, without having to introduce any C^*-algebraic framework or too much information on scattering theory. In fact, we shall keep the content of this section as simple as possible.

Let us start by considering the Hilbert space $\mathsf{L}^2(\mathbb{R}_+)$ and the Dirichlet Laplacian H_D on $\mathbb{R}_+ := (0,\infty)$. More precisely, we set $H_\mathrm{D} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ with the domain $\mathcal{D}(H_\mathrm{D}) = \{f \in \mathcal{H}^2(\mathbb{R}_+) \mid f(0) = 0\}$. Here $\mathcal{H}^2(\mathbb{R}_+)$ means the usual Sobolev space on $\mathbb{R}_+$ of order 2. For any $\alpha \in \mathbb{R}$, let us also consider the operator H^α defined by $H^\alpha = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ with $\mathcal{D}(H^\alpha) = \{f \in \mathcal{H}^2(\mathbb{R}_+) \mid f'(0) = \alpha f(0)\}$. It is well known that if $\alpha < 0$ the operator H^α possesses only one eigenvalue, namely $-\alpha^2$, and the corresponding eigenspace is generated by the function $x \mapsto \mathrm{e}^{\alpha x}$. On the other hand, for $\alpha \geq 0$ the operators H^α have no eigenvalue, and so does H_D.

As explained in the next section, a common object of scattering theory is defined by the following formula:

$$W_\pm^\alpha := s - \lim_{t\to\pm\infty} \mathrm{e}^{itH^\alpha}\, \mathrm{e}^{-itH_\mathrm{D}},$$

and this limit in the strong sense is known to exist for this model, see for example [57, Sec. 3.1]. Moreover, we shall provide below a very explicit formula for these operators. For that purpose, we need to introduce one more operator which is going to play a key role in the sequel. More precisely, we consider the unitary group $\{U_t\}_{t\in\mathbb{R}}$ acting on any $f \in \mathsf{L}^2(\mathbb{R}_+)$ as

$$[U_t f](x) = \mathrm{e}^{t/2} f\big(\mathrm{e}^t x\big), \qquad \forall x \in \mathbb{R}_+ \tag{2.1}$$

which is usually called *the unitary group of dilations*, and denote its self-adjoint generator by A and call it *the generator of dilations*.

Our first result for this model then reads.

Lemma 2.1. *For any $\alpha \in \mathbb{R}$, the following formula holds:*

$$W_-^\alpha = 1 + \tfrac{1}{2}\big(1 + \tanh(\pi A) - i\cosh(\pi A)^{-1}\big)\left[\frac{\alpha + i\sqrt{H_\mathrm{D}}}{\alpha - i\sqrt{H_\mathrm{D}}} - 1\right]. \tag{2.2}$$

Note that a similar formula for W_+^α also holds for this model, see Lemma 9.1. Since the proof of this lemma has never appeared in the literature, we provide it in the Appendix. Motivated by the above formula, let us now introduce the function

$$\Gamma^\alpha_\blacksquare : [0,+\infty] \times [-\infty,+\infty] \to \mathbb{C}$$
$$(x,y) \mapsto 1 + \tfrac{1}{2}\big(1+\tanh(\pi y) - i\cosh(\pi y)^{-1}\big)\left[\frac{\alpha + i\sqrt{x}}{\alpha - i\sqrt{x}} - 1\right].$$

Since this function is continuous on the square $\blacksquare := [0,+\infty] \times [-\infty,+\infty]$, its restriction on the boundary $\square$ of the square is also well defined and continuous. Note that this boundary is made of four parts: $\square = B_1 \cup B_2 \cup B_3 \cup B_4$ with $B_1 = \{0\} \times [-\infty,+\infty]$, $B_2 = [0,+\infty] \times \{+\infty\}$, $B_3 = \{+\infty\} \times [-\infty,+\infty]$, and $B_4 = [0,+\infty] \times \{-\infty\}$. Thus, the algebra $C(\square)$ of continuous functions on $\square$ can be viewed as a subalgebra of

$$C\big([-\infty,+\infty]\big) \oplus C\big([0,+\infty]\big) \oplus C\big([-\infty,+\infty]\big) \oplus C\big([0,+\infty]\big) \tag{2.3}$$

given by elements $\Gamma = (\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4)$ which coincide at the corresponding end points, that is,

$$\Gamma_1(+\infty) = \Gamma_2(0),\ \Gamma_2(+\infty) = \Gamma_3(+\infty),\ \Gamma_3(-\infty) = \Gamma_4(+\infty),$$
$$\text{and } \Gamma_4(0) = \Gamma_1(-\infty).$$

With these notations, the restriction function $\Gamma^\alpha_\square := \Gamma^\alpha_\blacksquare\big|_\square$ is given for $\alpha \neq 0$ by

$$\Gamma^\alpha_\square = \Big(1, \frac{\alpha + i\sqrt{\cdot}}{\alpha - i\sqrt{\cdot}}, -\tanh(\pi\cdot) + i\cosh(\pi\cdot)^{-1}, 1\Big) \tag{2.4}$$

and for $\alpha = 0$ by

$$\Gamma^0_\square := \Big(-\tanh(\pi\cdot) + i\cosh(\pi\cdot)^{-1}, -1, -\tanh(\pi\cdot) + i\cosh(\pi\cdot)^{-1}, 1\Big). \tag{2.5}$$

For simplicity, we have directly written this function in the representation provided by (2.3).

Let us now observe that the boundary $\square$ of $\blacksquare$ is homeomorphic to the circle $\mathbb{S}$. Observe in addition that the function $\Gamma^\alpha_\square$ takes its values in the unit circle $\mathbb{T}$ of $\mathbb{C}$. Then, since $\Gamma^\alpha_\square$ is a continuous function on the closed curve $\square$ and takes values in $\mathbb{T}$, its winding number $\mathrm{Wind}(\Gamma^\alpha_\square)$ is well defined and can easily be computed. So, let us compute separately the contribution $w_j(\Gamma^\alpha_\square)$ to this winding number on each component B_j of $\square$. By convention, we shall turn around $\square$ clockwise, starting from the left-down corner, and the increase in the winding number is also counted clockwise. Let us stress that the contribution on B_3 has to be computed from $+\infty$ to $-\infty$, and the contribution on B_4 from $+\infty$ to 0. Without difficulty one gets:

	$w_1(\Gamma^\alpha_\square)$	$w_2(\Gamma^\alpha_\square)$	$w_3(\Gamma^\alpha_\square)$	$w_4(\Gamma^\alpha_\square)$	$\mathrm{Wind}(\Gamma^\alpha_\square)$
$\alpha < 0$	0	1/2	1/2	0	1
$\alpha = 0$	−1/2	0	1/2	0	0
$\alpha > 0$	0	−1/2	1/2	0	0

By comparing the last column of this table with the information on the eigenvalues of H^α mentioned at the beginning of the section one gets:

Proposition 2.2. *For any $\alpha \in \mathbb{R}$ the following equality holds:*

$$\mathrm{Wind}(\Gamma^\alpha_\square) = \text{ number of eigenvalues of } H^\alpha. \tag{2.6}$$

The content of this proposition is an example of Levinson's theorem. Indeed, it relates the number of bound states of the operator H^α to a quantity computed on the scattering part of the system. Let us already mention that the contribution $w_2(\Gamma^\alpha_\square)$ is the only one usually considered in the literature. However, we can immediately observe that if $w_1(\Gamma^\alpha_\square)$ and $w_3(\Gamma^\alpha_\square)$ are disregarded, then no meaningful statement can be obtained.

Obviously, the above result should now be recast in a more general framework. Indeed, except for very specific models, it is usually not possible to compute precisely both sides of (2.6), but our aim is to show that such an equality still holds in a much more general setting. For that purpose, a C^*-algebraic framework will be constructed in Section 4.

3. Scattering theory: a brief introduction

In this section, we introduce the main objects of spectral and scattering theory which will be used throughout this paper.

Let us start by recalling a few basic facts from spectral theory. We consider a separable Hilbert space $\mathcal{H}$, with its scalar product denoted by $\langle \cdot, \cdot \rangle$ and its norm by $\|\cdot\|$. The set of bounded linear operators on $\mathcal{H}$ is denoted by $\mathcal{B}(\mathcal{H})$. Now, if $\mathcal{B}(\mathbb{R})$ denotes the set of Borel sets in $\mathbb{R}$ and if $\mathcal{P}(\mathcal{H})$ denotes the set of orthogonal projections on $\mathcal{H}$, then *a spectral measure* is a map $E : \mathcal{B}(\mathbb{R}) \to \mathcal{P}(\mathcal{H})$ satisfying the following properties:

(i) $E(\emptyset) = 0$ and $E(\mathbb{R}) = 1$,

(ii) If $\{\vartheta_n\}_{n\in\mathbb{N}}$ is a family of disjoint Borel sets, then $E(\cup_n \vartheta_n) = \sum_n E(\vartheta_n)$ (convergence in the strong topology).

The importance of spectral measures comes from their relation with the set of self-adjoint operators in $\mathcal{H}$. More precisely, let H be a self-adjoint operator acting in $\mathcal{H}$, with its domain denoted by $\mathcal{D}(H)$. Then, there exists a unique spectral measure $E(\cdot)$ such that $H = \int_\mathbb{R} \lambda E(\mathrm{d}\lambda)$. Note that this integral has to be understood in the strong sense, and only on elements of $\mathcal{D}(H)$.

This measure can now be decomposed into three parts, namely its absolutely continuous part, its singular continuous part, and its pure point part. More precisely, there exists a decomposition of the Hilbert space $\mathcal{H} = \mathcal{H}_{\mathrm{ac}}(H) \oplus \mathcal{H}_{\mathrm{sc}}(H) \oplus \mathcal{H}_{\mathrm{p}}(H)$ (which depends on H) such that for any $f \in \mathcal{H}_\bullet(H)$, the measure

$$\mathcal{B}(\mathbb{R}) \ni \vartheta \mapsto \langle E(\vartheta)f, f\rangle \in \mathbb{R}$$

is of the type $\bullet$, *i.e.*, absolutely continuous, singular continuous or pure point. It follows that the operator H is reduced by this decomposition of the Hilbert space, *i.e.*, $H = H_{\rm ac} \oplus H_{\rm sc} \oplus H_{\rm p}$. In other words, if one sets $E_{\rm ac}(H)$, $E_{\rm sc}(H)$ and $E_{\rm p}(H)$ for the orthogonal projections on $\mathcal{H}_{\rm ac}(H)$, $\mathcal{H}_{\rm sc}(H)$ and $\mathcal{H}_{\rm p}(H)$ respectively, then these projections commute with H and one has $H_{\rm ac} = HE_{\rm ac}(H)$, $H_{\rm sc} = HE_{\rm sc}(H)$ and $H_{\rm p} = HE_{\rm p}(H)$. In addition, if $\sigma(H)$ denotes the spectrum of the operator H, we then set $\sigma_{\rm ac}(H) := \sigma(H_{\rm ac})$, $\sigma_{\rm sc}(H) := \sigma(H_{\rm sc})$, and if $\sigma_{\rm p}(H)$ denotes the set of eigenvalues of H, then the equality $\overline{\sigma_{\rm p}(H)} = \sigma(H_{\rm p})$ holds. In this framework the operator H is said to be purely absolutely continuous if $\mathcal{H}_{\rm sc}(H) = \mathcal{H}_{\rm p}(H) = \{0\}$, or is said to have a finite point spectrum (counting multiplicity) if $\dim\big(\mathcal{H}_{\rm p}(H)\big) < \infty$. In this case, we also write $\sharp\sigma_p(H) < \infty$.

Let us now move to scattering theory. It is a comparison theory, therefore we have to consider two self-adjoint operators H_0 and H in the Hilbert space $\mathcal{H}$. A few requirements will be imposed on these operators and on their relationships. Let us first state these conditions, and discuss them afterwards.

Assumption 3.1. *The following conditions hold for H_0 and H:*

(i) *H_0 is purely absolutely continuous,*
(ii) $\sharp\sigma_p(H) < \infty$,
(iii) *the wave operators* $W_\pm := s - \lim_{t\to\pm\infty} e^{itH}\, e^{-itH_0}$ *exist,*
(iv) $\mathrm{Ran}(W_-) = \mathrm{Ran}(W_+) = \mathcal{H}_p(H)^\perp = \big(1 - E_{\rm p}(H)\big)\mathcal{H}$.

The assumption (i) is a rather common condition in scattering theory. Indeed, since H_0 is often thought as a comparison operator, we expect it to be as simple as possible. For that reason, any eigenvalue for H_0 is automatically ruled out. For the same reason, we will assume that H_0 does not possess a singular continuous part. On the other hand, assumption (ii), which imposes that the point spectrum of H is finite (multiplicity included) is certainly restrictive, but is natural for our purpose. Indeed, since at the end of the day we are looking for a relation involving the number of bound states, the resulting equality is meaningful only if such a number is finite.

Assumption (iii) is the main condition on the relation between H_0 and H. In fact, this assumption does not directly compare these two operators, but compare their respective evolution group $\{e^{-itH_0}\}_{t\in\mathbb{R}}$ and $\{e^{-itH}\}_{t\in\mathbb{R}}$ for $|t|$ large enough. This condition is usually rephrased as *the existence of the wave operators*. Note that $s - \lim$ means the limit in the strong sense, *i.e.*, when these operators are applied on an element of the Hilbert space. For a concrete model, checking this existence is a central part of scattering theory, and can be a rather complicated task. We shall see in the examples developed later on that this condition can be satisfied if H corresponds to a suitable perturbation of H_0. For the time being, imposing this existence corresponds in fact to the weakest condition necessary for the subsequent construction. Finally, assumption (iv) is usually called *the asymptotic completeness* of the wave operators. It is a rather natural expectation in the setting of scattering theory. In addition, since $\mathrm{Ran}(W_\pm) \subset \mathcal{H}_{\rm ac}(H)$ always holds, this assumption implies in particular that H has no singular continuous spectrum, *i.e.*, $\mathcal{H}_{\rm sc}(H) = \{0\}$. The main idea behind this notion of asymptotic completeness will be explained in Remark 3.2.

Let us now stress some important consequences of Assumption 3.1. Firstly, the wave operators $W_\pm$ are isometries, with

$$W_\pm^* W_\pm = 1 \quad \text{and} \quad W_\pm W_\pm^* = 1 - E_{\mathrm{p}}(H), \tag{3.1}$$

where * means the adjoint operator. Secondly, $W_\pm$ are Fredholm operators and satisfy the so-called *intertwining relation*, namely $W_\pm \,\mathrm{e}^{-itH_0} = \mathrm{e}^{-itH}\, W_\pm$ for any $t \in \mathbb{R}$. Another crucial consequence of our assumptions is that *the scattering operator*

$$S := W_+^* W_-$$

is unitary and commute with H_0, *i.e.*, the relation $S\,\mathrm{e}^{-itH_0} = \mathrm{e}^{-itH_0}\, S$ holds for any $t \in \mathbb{R}$. Note that this latter property means that S and H_0 can be decomposed simultaneously. More precisely, from the general theory of self-adjoint operators, there exists a unitary map $\mathscr{F}_0 : \mathcal{H} \to \int_{\sigma(H_0)}^{\oplus} \mathcal{H}(\lambda)\,\mathrm{d}\lambda$ from $\mathcal{H}$ to a direct integral Hilbert space such that $\mathscr{F}_0 H_0 \mathscr{F}_0^* = \int_{\sigma(H_0)}^{\oplus} \lambda\,\mathrm{d}\lambda$. Then, the mentioned commutation relation implies that

$$\mathscr{F}_0 S \mathscr{F}_0^* = \int_{\sigma(H_0)}^{\oplus} S(\lambda)\,\mathrm{d}\lambda$$

with $S(\lambda)$ a unitary operator in the Hilbert space $\mathcal{H}(\lambda)$ for almost every λ. The operator $S(\lambda)$ is usually called *the scattering matrix at energy* λ, even when this operator is not a matrix but an operator acting in a infinite-dimensional Hilbert space.

Remark 3.2. In order to understand the idea behind the asymptotic completeness, let us assume it and consider any $f \in \mathcal{H}_{\mathrm{ac}}(H)$. We then set $f_\pm := W_\pm^* f$ and observe that

$$\begin{aligned}\lim_{t\to\pm\infty} \big\| \mathrm{e}^{-itH} f - \mathrm{e}^{-itH_0} f_\pm \big\| &= \lim_{t\to\pm\infty} \big\| f - \mathrm{e}^{itH}\, \mathrm{e}^{-itH_0} f_\pm \big\| \\ &= \lim_{t\to\pm\infty} \big\| f - \mathrm{e}^{itH}\, \mathrm{e}^{-itH_0} W_\pm^* f \big\| \\ &= 0,\end{aligned}$$

where the second equality in (3.1) together with the equality $1 - E_{\mathrm{p}}(H) = E_{\mathrm{ac}}(H)$ have been used for the last equality. Thus, the asymptotic completeness of the wave operators means that for any $f \in \mathcal{H}_{\mathrm{p}}(H)^\perp$ the element $\mathrm{e}^{-itH} f$ can be well approximated by the simpler expression $\mathrm{e}^{-itH_0} f_\pm$ for t going to $\pm\infty$. As already mentioned, one usually considers the operator H_0 simpler than H, and for that reason the evolution group $\{\mathrm{e}^{-itH_0}\}_{t\in\mathbb{R}}$ is considered simpler than the evolution group $\{\mathrm{e}^{-itH}\}_{t\in\mathbb{R}}$.

4. The C^*-algebraic framework

In this section we introduce the C^*-algebraic framework which is necessary for interpreting Levinson's theorem as an index theorem. We start by defining the K-groups for a C^*-algebra.

4.1. The K-groups

Our presentation of the K-groups is mainly based the first chapters of the book [50] to which we refer for details.

For any C^*-algebra $\mathcal{E}$, let us denote by $\mathcal{M}_n(\mathcal{E})$ the set of all $n \times n$ matrices with entries in $\mathcal{E}$. Addition, multiplication and involution for such matrices are mimicked from the scalar case, *i.e.*, when $\mathcal{E} = \mathbb{C}$. For defining a C^*-norm on $\mathcal{M}_n(\mathcal{E})$, consider any injective $*$-morphism $\phi : \mathcal{E} \to \mathcal{B}(\mathcal{H})$ for some Hilbert space $\mathcal{H}$, and extend this morphism to a morphism $\phi : \mathcal{M}_n(\mathcal{E}) \to \mathcal{B}(\mathcal{H}^n)$ by defining

$$\phi \begin{pmatrix} a_{11} & \dots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \dots & a_{nn} \end{pmatrix} \begin{pmatrix} f_1 \\ \vdots \\ f_n \end{pmatrix} = \begin{pmatrix} \phi(a_{11})f_1 + \cdots + \phi(a_{1n})f_n \\ \vdots \\ \phi(a_{n1})f_1 + \cdots + \phi(a_{nn})f_n \end{pmatrix} \tag{4.1}$$

for any ${}^t(f_1, \dots, f_n) \in \mathcal{H}^n$ (the notation ${}^t(\dots)$ means the transpose of a vector). Then a C^*-norm on $\mathcal{M}_n(\mathcal{E})$ is obtained by setting $\|a\| := \|\phi(a)\|$ for any $a \in \mathcal{M}_n(\mathcal{E})$, and this norm is independent of the choice of ϕ.

In order to construct the first K-group associated with $\mathcal{E}$, let us consider the set

$$\mathcal{P}_\infty(\mathcal{E}) = \bigcup_{n \in \mathbb{N}} \mathcal{P}_n(\mathcal{E})$$

with $\mathcal{P}_n(\mathcal{E}) := \{p \in \mathcal{M}_n(\mathcal{E}) \mid p = p^* = p^2\}$. Such an element p is called a projection. $\mathcal{P}_\infty(\mathcal{E})$ is then endowed with a relation, namely for $p \in \mathcal{P}_n(\mathcal{E})$ and $q \in \mathcal{P}_m(\mathcal{E})$ one writes $p \sim_0 q$ if there exists $v \in \mathcal{M}_{m,n}(\mathcal{E})$ such that $p = v^*v$ and $q = vv^*$. Clearly, $\mathcal{M}_{m,n}(\mathcal{E})$ denotes the set of $m \times n$ matrices with entries in $\mathcal{E}$, and the adjoint v^* of $v \in \mathcal{M}_{m,n}(\mathcal{E})$ is obtained by taking the transpose of the matrix, and then the adjoint of each entry. This relation defines an equivalence relation which combines the Murray–von Neumann equivalence relation together with an identification of projections in different sized matrix algebras over $\mathcal{E}$. We also endow $\mathcal{P}_\infty(\mathcal{E})$ with a binary operation, namely if $p, q \in \mathcal{P}_\infty(\mathcal{E})$ we set $p \oplus q = \left(\begin{smallmatrix} p & 0 \\ 0 & q \end{smallmatrix}\right)$ which is again an element of $\mathcal{P}_\infty(\mathcal{E})$.

We can then define the quotient space

$$\mathcal{D}(\mathcal{E}) := \mathcal{P}_\infty(\mathcal{E}) / \sim_0$$

with its elements denoted by $[p]$ (the equivalence class containing $p \in \mathcal{P}_\infty(\mathcal{E})$). One also sets

$$[p] + [q] := [p \oplus q]$$

for any $p, q \in \mathcal{P}_\infty(\mathcal{E})$, and it turns out that the pair $\big(\mathcal{D}(\mathcal{E}), +\big)$ defines an Abelian semigroup.

In order to obtain an Abelian group from the semigroup, let us recall that there exists a canonical construction which allows one to add "the opposites" to any Abelian semigroup and which is called *the Grothendieck construction*. More precisely, for an Abelian semigroup $(\mathcal{D}, +)$ we consider on $\mathcal{D} \times \mathcal{D}$ an equivalence relation, namely $(a_1, b_1) \sim (a_2, b_2)$ if there exists $c \in \mathcal{D}$ such that $a_1 + b_2 + c =$

$a_2 + b_1 + c$. The elements of the quotient $\mathcal{D} \times \mathcal{D}/\sim$ are denoted by $\langle a, b\rangle$ and this quotient corresponds to an Abelian group with the addition

$$\langle a_1, b_1\rangle + \langle a_2, b_2\rangle := \langle a_1 + a_2, b_1 + b_2\rangle.$$

One readily checks that the equalities $-\langle a, b\rangle = \langle b, a\rangle$ and $\langle a, a\rangle = 0$ hold. This group is called *the Grothendieck group* associated with $(\mathcal{D}, +)$ and is denoted by $\big(\mathcal{G}(\mathcal{D}), +\big)$.

Coming back to a unital C^*-algebra $\mathcal{E}$, we set

$$K_0(\mathcal{E}) := \mathcal{G}\big(\mathcal{D}(\mathcal{E})\big),$$

which is thus an Abelian group with the binary operation $+$, and define the map $[\cdot]_0 : \mathcal{P}_\infty(\mathcal{E}) \to K_0(\mathcal{E})$ by $[p]_0 := \langle [p] + [q], [q]\rangle$ for an arbitrary fixed $q \in \mathcal{P}_\infty(\mathcal{E})$. Note that this latter map is called the *Grothendieck map* and is independent of the choice of q. Note also that an alternative description of $K_0(\mathcal{E})$ is provided by differences of equivalence classes of projections, *i.e.*,

$$K_0(\mathcal{E}) = \big\{[p]_0 - [q]_0 \mid p, q \in \mathcal{P}_\infty(\mathcal{E})\big\}. \tag{4.2}$$

At the end of the day, we have thus obtained an Abelian group $\big(K_0(\mathcal{E}), +\big)$ canonically associated with the unital C^*-algebra $\mathcal{E}$ and which is essentially made of equivalence classes of projections.

Before discussing the non-unital case, let us observe that if $\mathcal{E}_1$, $\mathcal{E}_2$ are unital C^*-algebras, and if $\phi : \mathcal{E}_1 \to \mathcal{E}_2$ is a $*$-morphism, then ϕ extends to a $*$-morphism $\mathcal{M}_n(\mathcal{E}_1) \to \mathcal{M}_n(\mathcal{E}_2)$, as already mentioned just before (4.1). Since a $*$-morphism maps projections to projections, it follows that ϕ maps $\mathcal{P}_\infty(\mathcal{E}_1)$ into $\mathcal{P}_\infty(\mathcal{E}_2)$. One can then infer from the universal property of the K_0-groups that ϕ defines a group homomorphism $K_0(\phi) : K_0(\mathcal{E}_1) \to K_0(\mathcal{E}_2)$ given by

$$K_0(\phi)([p]_0) = [\phi(p)]_0 \qquad \forall p \in \mathcal{P}_\infty(\mathcal{E}_1).$$

The existence of this morphism will be necessary right now.

If $\mathcal{E}$ is not unital, the construction is slightly more involved. Recall first that with any C^*-algebra $\mathcal{E}$ (with or without a unit) one can associate a unique unital C^*-algebra $\mathcal{E}^+$ that contains $\mathcal{E}$ as an ideal, and such that the quotient $\mathcal{E}^+/\mathcal{E}$ is isomorphic to $\mathbb{C}$. We do not provide here this explicit construction, but refer to [50, Ex. 1.3] for a detailed presentation. However, let us mention the fact that the short exact sequence[2]

$$0 \longrightarrow \mathcal{E} \longrightarrow \mathcal{E}^+ \xrightarrow{\pi} \mathbb{C} \longrightarrow 0$$

is split exact, in the sense that if one sets $\lambda : \mathbb{C} \ni \alpha \mapsto \alpha 1_{\mathcal{E}^+} \in \mathcal{E}^+$, then λ is a $*$-morphism and the equality $\pi\big(\lambda(\alpha)\big) = \alpha$ holds for any $\alpha \in \mathbb{C}$. Observe now that since $\pi : \mathcal{E}^+ \to \mathbb{C}$ is a $*$-morphism between unital C^*-algebras, it follows from the construction made in the previous paragraph that there exists a group morphism $K_0(\pi) : K_0(\mathcal{E}^+) \to K_0(\mathbb{C})$. In the case of a non-unital C^*-algebra $\mathcal{E}$, we set $K_0(\mathcal{E})$

[2] A short exact sequence of C^*-algebras $0 \to \mathcal{J} \xrightarrow{\iota} \mathcal{E} \xrightarrow{q} \mathcal{Q} \to 0$ consists in three C^*-algebras $\mathcal{J}, \mathcal{E}$ and $\mathcal{Q}$ and two $*$-morphisms ι and q such that $\mathrm{Im}(\iota) = \mathrm{Ker}(q)$ and such that ι is injective while q is surjective.

for the kernel of this morphism $K_0(\pi)$, which is obviously an Abelian group with the binary operation of $K_0(\mathcal{E}^+)$. In summary:

$$K_0(\mathcal{E}) := \mathrm{Ker}\Big(K_0(\pi) : K_0(\mathcal{E}^+) \to K_0(\mathbb{C})\Big)$$

which is an Abelian group once endowed with the binary operation $+$ inherited from $K_0(\mathcal{E}^+)$.

Let us still provide an alternative description of $K_0(\mathcal{E})$, in a way similar to the one provided in (4.2), but which holds both in the unital and in the non-unital case. For that purpose, let us introduce the scalar mapping $s : \mathcal{E}^+ \to \mathcal{E}^+$ obtained by the composition $\lambda \circ \pi$. Note that $\pi\big(s(a)\big) = \pi(a)$ and that $a - s(a)$ belongs to $\mathcal{E}$ for any $a \in \mathcal{E}^+$. As before, we keep the same notation for the extension of s to $\mathcal{M}_n(\mathcal{E}^+)$. With these notations, one has for any C^*-algebra $\mathcal{E}$:

$$K_0(\mathcal{E}) = \big\{[p]_0 - [s(p)]_0 \mid p \in \mathcal{P}_\infty(\mathcal{E}^+)\big\}.$$

In summary, for any C^*-algebra (with or without unit) we have constructed an Abelian group consisting essentially of equivalence classes of projections. Since projections are not the only special elements in a C^*-algebra $\mathcal{E}$, it is natural to wonder if an analogous construction holds for other families of elements of $\mathcal{E}$? The answer is yes, for families of unitary elements of $\mathcal{E}$, and fortunately this new construction is simpler. The resulting Abelian group will be denoted by $K_1(\mathcal{E})$, and we are now going to describe how to obtain it.

In order to construct the second K-group associated with a unital C^*-algebra $\mathcal{E}$, let us consider the set

$$\mathcal{U}_\infty(\mathcal{E}) = \bigcup_{n\in\mathbb{N}} \mathcal{U}_n(\mathcal{E})$$

with $\mathcal{U}_n(\mathcal{E}) := \{u \in \mathcal{M}_n(\mathcal{E}) \mid u^* = u^{-1}\}$. This set is endowed with a binary operation, namely if $u, v \in \mathcal{U}_\infty(\mathcal{E})$ we set $u \oplus v = \left(\begin{smallmatrix} u & 0 \\ 0 & v \end{smallmatrix}\right)$ which is again an element of $\mathcal{U}_\infty(\mathcal{E})$. We also introduce an equivalence relation on $\mathcal{U}_\infty(\mathcal{E})$: if $u \in \mathcal{U}_n(\mathcal{E})$ and $v \in \mathcal{U}_m(\mathcal{E})$, one sets $u \sim_1 v$ if there exists a natural number $k \geq \max\{m, n\}$ such that $u \oplus 1_{k-n}$ is homotopic[3] to $v \oplus 1_{k-m}$ in $\mathcal{U}_k(\mathcal{E})$. Here we have used the notation 1_ℓ for the identity matrix[4] in $\mathcal{U}_\ell(\mathcal{E})$.

Based on this construction, for any C^*-algebra $\mathcal{E}$ one sets

$$K_1(\mathcal{E}) := \mathcal{U}_\infty(\mathcal{E}^+)/\sim_1,$$

and denotes the elements of $K_1(\mathcal{E})$ by $[u]_1$ for any $u \in \mathcal{U}_\infty(\mathcal{E}^+)$. $K_1(\mathcal{E})$ is naturally endowed with a binary operation, by setting for any $u, v \in \mathcal{U}_\infty(\mathcal{E}^+)$

$$[u]_1 + [v]_1 := [u \oplus v]_1,$$

[3]Recall that two elements $u_0, u_1 \in \mathcal{U}_k(\mathcal{E})$ are homotopic in $\mathcal{U}_k(\mathcal{E})$, written $u_0 \sim_h u_1$, if there exists a continuous map $u : [0,1] \ni t \mapsto u(t) \in \mathcal{U}_k(\mathcal{E})$ such that $u(0) = u_0$ and $u(1) = u_1$.

[4]The notation 1_n for the identity matrix in $\mathcal{M}_n(\mathcal{E})$ is sometimes very convenient, and sometimes very annoying (with 1 much preferable). In the sequel we shall use both conventions, and this should not lead to any confusion.

which is commutative and associative. Its zero element is provided by $[1]_1 := [1_n]_1$ for any natural number n, and one has $-[u]_1 = [u^*]_1$ for any $u \in \mathcal{U}_\infty(\mathcal{E}^+)$. As a consequence, $\big(K_1(\mathcal{E}), +\big)$ is an Abelian group, which corresponds to the second K-group of $\mathcal{E}$.

In summary, for any C^*-algebra we have constructed an Abelian group consisting essentially of equivalence classes of unitary elements. As a result, any C^*-algebra is intimately linked with two Abelian groups, one based on projections and one based on unitary elements. Before going to the next step of the construction, let us provide two examples of K-groups which can be figured out without difficulty.

Example 4.1.

(i) Let $C(\mathbb{S})$ denote the C^*-algebra of continuous functions on the unit circle $\mathbb{S}$, with the L^∞-norm, and let us identify this algebra with $\big\{\zeta \in C([0, 2\pi]) \mid \zeta(0) = \zeta(2\pi)\big\}$, also endowed with the L^∞-norm. Some unitary elements of $C(\mathbb{S})$ are provided for any $m \in \mathbb{Z}$ by the functions

$$\zeta_m : [0, 2\pi] \ni \theta \mapsto \mathrm{e}^{-im\theta} \in \mathbb{T}.$$

Clearly, for two different values of m the functions ζ_m are not homotopic, and thus define different classes in $K_1\big(C(\mathbb{S})\big)$. With some more efforts one can show that these elements define in fact all elements of $K_1\big(C(\mathbb{S})\big)$, and indeed one has

$$K_1\big(C(\mathbb{S})\big) \cong \mathbb{Z}.$$

Note that this isomorphism is implemented by the winding number $\mathrm{Wind}(\cdot)$, which is roughly defined for any continuous function on $\mathbb{S}$ with values in $\mathbb{T}$ as the number of times this function turns around 0 along the path from 0 to 2π. Clearly, for any $m \in \mathbb{Z}$ one has $\mathrm{Wind}(\zeta_m) = m$. More generally, if det denotes the determinant on $\mathcal{M}_n(\mathbb{C})$ then the mentioned isomorphism is given by $\mathrm{Wind} \circ \det$ on $\mathcal{U}_n\big(C(\mathbb{S})\big)$.

(ii) Let $\mathcal{K}(\mathcal{H})$ denote the C^*-algebra of all compact operators on a infinite-dimensional and separable Hilbert space $\mathcal{H}$. For any n one can consider the orthogonal projections on subspaces of dimension n of $\mathcal{H}$, and these finite-dimensional projections belong to $\mathcal{K}(\mathcal{H})$. It is then not too difficult to show that two projections of the same dimension are Murray–von Neumann equivalent, while projections corresponding to two different values of n are not. With some more efforts, one shows that the dimension of these projections plays the crucial role for the definition of $K_0\big(\mathcal{K}(\mathcal{H})\big)$, and one has again

$$K_0\big(\mathcal{K}(\mathcal{H})\big) \cong \mathbb{Z}.$$

In this case, the isomorphism is provided by the usual trace Tr on finite-dimensional projections, and by the tensor product of this trace with the trace tr on $\mathcal{M}_n(\mathbb{C})$. More precisely, on any element of $\mathcal{P}_n\big(\mathcal{K}(\mathcal{H})\big)$ the mentioned isomorphism is provided by $\mathrm{Tr} \circ \mathrm{tr}$.

4.2. The boundary maps

We shall now consider three C^*-algebras, with some relations between them. Since two K-groups can be associated with each of them, we can expect that the relations between the algebras have a counterpart between the K-groups. This is indeed the case.

Consider the short exact sequence of C^*-algebras

$$0 \to \mathcal{J} \overset{\iota}{\hookrightarrow} \mathcal{E} \overset{q}{\to} \mathcal{Q} \to 0 \tag{4.3}$$

where the notation $\hookrightarrow$ means that $\mathcal{J}$ is an ideal in $\mathcal{E}$, and therefore ι corresponds to the inclusion map. In this setting, $\mathcal{Q}$ corresponds either to the quotient $\mathcal{E}/\mathcal{J}$ or is isomorphic to this quotient. The relations between the K-groups of these algebras can then be summarized with the following six-term exact sequence

$$\begin{array}{ccccc} K_1(\mathcal{J}) & \longrightarrow & K_1(\mathcal{E}) & \longrightarrow & K_1(\mathcal{Q}) \\ {\scriptstyle\exp}\big\downarrow & & & & \big\downarrow{\scriptstyle\mathrm{ind}} \\ K_0(\mathcal{Q}) & \longrightarrow & K_0(\mathcal{E}) & \longrightarrow & K_0(\mathcal{J}) \ . \end{array}$$

In this diagram, each arrow corresponds to a group morphism, and the range of an arrow is equal to the kernel of the following one. Note that we have indicated the name of two special arrows, one is called *the exponential map*, and the other one *the index map*. These two arrows are generically called *boundary maps*. In this paper, we shall only deal with the index map, but let us mention that the exponential map has also played a central role for exhibiting other index theorems in the context of solid states physics [28, 34].

We shall not recall the construction of the index map in the most general framework, but consider a slightly restricted setting (see [50, Chap. 9] for a complete presentation). For that purpose, let us assume that the algebra $\mathcal{E}$ is unital, in which case $\mathcal{Q}$ is unital as well and the morphism q is unit preserving. Then, a reformulation of [50, Prop. 9.2.4.(ii)] in our context reads:

Proposition 4.2. *Consider the short exact sequence* (4.3) *with $\mathcal{E}$ unital. Assume that Γ is a unitary element of $\mathcal{M}_n(\mathcal{Q})$ and that there exists a partial isometry $W \in \mathcal{M}_n(\mathcal{E})$ such that $q(W) = \Gamma$. Then $1_n - W^*W$ and $1_n - WW^*$ are projections in $\mathcal{M}_n(\mathcal{J})$, and*

$$\mathrm{ind}([\Gamma]_1) = [1_n - W^*W]_0 - [1_n - WW^*]_0 \ .$$

Let us stress the interest of this statement. Starting from a unitary element Γ of $\mathcal{M}_n(\mathcal{Q})$, one can naturally associate to it an element of $K_0(\mathcal{J})$. In addition, since the elements of the K-groups are made of equivalence classes of objects, such an association is rather stable under small deformations.

Before starting with applications of this formalism to scattering systems, let us add one more reformulation of the previous proposition. The key point in the next statement is that the central role is played by the partial isometry W instead of the unitary element Γ. In fact, the following statement is at the root of our topological approach of Levinson's theorem.

Proposition 4.3. *Consider the short exact sequence* (4.3) *with* $\mathcal{E}$ *unital. Let* W *be a partial isometry in* $\mathcal{M}_n(\mathcal{E})$ *and assume that* $\Gamma := q(W)$ *is a unitary element of* $\mathcal{M}_n(\mathcal{Q})$*. Then* $1_n - W^*W$ *and* $1_n - WW^*$ *are projections in* $\mathcal{M}_n(\mathcal{J})$*, and*

$$\mathrm{ind}([q(W)]_1) = [1_n - W^*W]_0 - [1_n - WW^*]_0 \ .$$

4.3. The abstract topological Levinson theorem

Let us now add the different pieces of information we have presented so far, and get an abstract version of our Levinson theorem. For that purpose, we consider a separable Hilbert space $\mathcal{H}$ and a unital C^*-subalgebra $\mathcal{E}$ of $\mathcal{B}(\mathcal{H})$ which contains the ideal of $\mathcal{K}(\mathcal{H})$ of compact operators. We can thus look at the short exact sequence of C^*-algebras

$$0 \to \mathcal{K}(\mathcal{H}) \hookrightarrow \mathcal{E} \xrightarrow{q} \mathcal{E}/\mathcal{K}(\mathcal{H}) \to 0.$$

If we assume in addition that $\mathcal{E}/\mathcal{K}(\mathcal{H})$ is isomorphic to $C(\mathbb{S})$, and if we take the results presented in Example 4.1 into account, one infers that

$$\mathbb{Z} \cong K_1\big(C(\mathbb{S})\big) \xrightarrow{\mathrm{ind}} K_0\big(\mathcal{K}(\mathcal{H})\big) \cong \mathbb{Z}$$

with the first isomorphism realized by the winding number and the second isomorphism realized by the trace. As a consequence, one infers from this together with Proposition 4.3 that there exists $n \in \mathbb{Z}$ such that for any partial isometry $W \in \mathcal{E}$ with unitary $\Gamma := q(W) \in C(\mathbb{S})$ the following equality holds:

$$\mathrm{Wind}(\Gamma) = n\mathrm{Tr}\big([1 - W^*W] - [1 - WW^*]\big).$$

We emphasize once again that the interest in this equality is that the left-hand side is independent of the choice of any special representative in $[\Gamma]_1$. Let us also mention that the number n depends on the choice of the extension of $\mathcal{K}(\mathcal{H})$ by $C(\mathbb{S})$, see [56, Chap. 3.2], but also on the convention chosen for the computation of the winding number.

If we summarize all this in a single statement, one gets:

Theorem 4.4 (Abstract topological Levinson theorem). *Let* $\mathcal{H}$ *be a separable Hilbert space, and let* $\mathcal{E} \subset \mathcal{B}(\mathcal{H})$ *be a unital* C^**-algebra such that* $\mathcal{K}(\mathcal{H}) \subset \mathcal{E}$ *and* $\mathcal{E}/\mathcal{K}(\mathcal{H}) \cong C(\mathbb{S})$ (*with quotient morphism denoted by* q). *Then there exists* $n \in \mathbb{Z}$ *such that for any partial isometry* $W \in \mathcal{E}$ *with unitary* $\Gamma := q(W) \in C(\mathbb{S})$ *the following equality holds:*

$$\mathrm{Wind}(\Gamma) = n\mathrm{Tr}\big([1 - W^*W] - [1 - WW^*]\big). \tag{4.4}$$

In particular if $W = W_-$ *for some scattering system satisfying Assumption* 3.1*, the previous equality reads*

$$\mathrm{Wind}\big(q(W_-)\big) = -n\mathrm{Tr}\big([E_{\mathrm{p}}]\big).$$

Note that in applications, the factor n will be determined by computing both sides of the equality on an explicit example.

4.4. The leading example

We shall now provide a concrete short exact sequence of C^*-algebras, and illustrate the previous constructions on this example.

In the Hilbert space $\mathsf{L}^2(\mathbb{R})$ we consider the two canonical self-adjoint operators X of multiplication by the variable, and $D = -i\frac{\mathrm{d}}{\mathrm{d}x}$ of differentiation. These operators satisfy the canonical commutation relation written formally $[iD, X] = 1$, or more precisely $\mathrm{e}^{-isX}\,\mathrm{e}^{-itD} = \mathrm{e}^{-ist}\,\mathrm{e}^{-itD}\,\mathrm{e}^{-isX}$. We recall that the spectrum of both operators is $\mathbb{R}$. Then, for any functions $\varphi, \eta \in \mathsf{L}^\infty(\mathbb{R})$, one can consider by bounded functional calculus the operators $\varphi(X)$ and $\eta(D)$ in $\mathcal{B}\big(\mathsf{L}^2(\mathbb{R})\big)$. And by mixing some operators $\varphi_i(X)$ and $\eta_i(D)$ for suitable functions φ_i and η_i, we are going to produce an algebra $\mathcal{E}$ which will be useful in many applications. In fact, the first algebras which we are going to construct have been introduced in [19] for a different purpose, and these algebras have been an important source of inspiration for us. We also mention that related algebras had already been introduced a long time ago in [8, 9, 13, 14].

Let us consider the closure in $\mathcal{B}\big(\mathsf{L}^2(\mathbb{R})\big)$ of the $*$-algebra generated by elements of the form $\varphi_i(D)\eta_i(X)$, where φ_i, η_i are continuous functions on $\mathbb{R}$ which have limits at $\pm\infty$. Stated differently, φ_i, η_i belong to $C([-\infty, +\infty])$. Note that this algebra is clearly unital. In the sequel, we shall use the following notation:

$$\mathcal{E}_{(D,X)} := C^*\Big(\varphi_i(D)\eta_i(X) \mid \varphi_i, \eta_i \in C([-\infty, +\infty])\Big).$$

Let us also consider the C^*-algebra generated by $\varphi_i(D)\eta_i(X)$ with $\varphi_i, \eta_i \in C_0(\mathbb{R})$, which means that these functions are continuous and vanish at $\pm\infty$. As easily observed, this algebra is a closed ideal in $\mathcal{E}_{(D,X)}$ and is equal to the C^*-algebra $\mathcal{K}\big(\mathsf{L}^2(\mathbb{R})\big)$ of compact operators in $\mathsf{L}^2(\mathbb{R})$, see for example [19, Corol. 2.18].

Implicitly, the description of the quotient $\mathcal{E}_{(D,X)}/\mathcal{K}\big(\mathsf{L}^2(\mathbb{R})\big)$ has already been provided in Section 2. Let us do it more explicitly now. We consider the square $\blacksquare := [-\infty, +\infty] \times [-\infty, +\infty]$ whose boundary $\square$ is the union of four parts: $\square = C_1 \cup C_2 \cup C_3 \cup C_4$, with $C_1 = \{-\infty\} \times [-\infty, +\infty]$, $C_2 = [-\infty, +\infty] \times \{+\infty\}$, $C_3 = \{+\infty\} \times [-\infty, +\infty]$ and $C_4 = [-\infty, +\infty] \times \{-\infty\}$. We can also view $C(\square)$ as the subalgebra of

$$C([-\infty, +\infty]) \oplus C([-\infty, +\infty]) \oplus C([-\infty, +\infty]) \oplus C([-\infty, +\infty]) \tag{4.5}$$

given by elements $\Gamma := (\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4)$ which coincide at the corresponding end points, that is, $\Gamma_1(+\infty) = \Gamma_2(-\infty)$, $\Gamma_2(+\infty) = \Gamma_3(+\infty)$, $\Gamma_3(-\infty) = \Gamma_4(+\infty)$, and $\Gamma_4(-\infty) = \Gamma_1(-\infty)$. Then $\mathcal{E}_{(D,X)}/\mathcal{K}\big(\mathsf{L}^2(\mathbb{R})\big)$ is isomorphic to $C(\square)$, and if we denote the quotient map by

$$q : \mathcal{E}_{(D,X)} \to \mathcal{E}_{(D,X)}/\mathcal{K}\big(\mathsf{L}^2(\mathbb{R})\big) \cong C(\square)$$

then the image $q\big(\varphi(D)\eta(X)\big)$ in (4.5) is given by $\Gamma_1 = \varphi(-\infty)\eta(\cdot)$, $\Gamma_2 = \varphi(\cdot)\eta(+\infty)$, $\Gamma_3 = \varphi(+\infty)\eta(\cdot)$ and $\Gamma_4 = \varphi(\cdot)\eta(-\infty)$. Note that this isomorphism is proved in [19, Thm. 3.22]. In summary, we have obtained the short exact sequence

$$0 \to \mathcal{K}\big(\mathsf{L}^2(\mathbb{R})\big) \hookrightarrow \mathcal{E}_{(D,X)} \xrightarrow{q} C(\square) \to 0$$

with $\mathcal{K}\big(\mathsf{L}^2(\mathbb{R})\big)$ and $\mathcal{E}_{(D,X)}$ represented in $\mathcal{B}\big(\mathsf{L}^2(\mathbb{R})\big)$, but with $C(\square)$ which is not naturally represented in $\mathcal{B}\big(\mathsf{L}^2(\mathbb{R})\big)$. Note however that each of the four functions summing up in an element of $C(\square)$ can individually be represented in $\mathcal{B}\big(\mathsf{L}^2(\mathbb{R})\big)$, either as a multiplication operator or as a convolution operator.

We shall now construct several isomorphic versions of these algebras. Indeed, if one looks back at the baby model, the wave operator is expressed in (2.2) with bounded functions of the two operators H_{D} and A, but not in terms of D and X. In fact, we shall first use a third pair of operators, namely L and A, acting in $\mathsf{L}^2(\mathbb{R}_+)$, and then come back to the pair (H_{D}, A) also acting in $\mathsf{L}^2(\mathbb{R}_+)$.

Let us consider the Hilbert space $\mathsf{L}^2(\mathbb{R}_+)$, and as in (2.1) the action of the dilation group with generator A. Let also B be the operator of multiplication in $\mathsf{L}^2(\mathbb{R}_+)$ by the function $-\ln$, *i.e.*, $[Bf](\lambda) = -\ln(\lambda)f(\lambda)$ for any $f \in C_{\mathrm{c}}(\mathbb{R}_+)$ and $\lambda \in \mathbb{R}_+$. Note that if one sets L for the self-adjoint operator of multiplication by the variable in $\mathsf{L}^2(\mathbb{R}_+)$, *i.e.*,

$$[Lf](\lambda) := \lambda f(\lambda) \qquad f \in C_{\mathrm{c}}(\mathbb{R}_+) \text{ and } \lambda \in \mathbb{R}_+, \tag{4.6}$$

then one has $B = -\ln(L)$. Now, the equality $[iB, A] = 1$ holds (once suitably defined), and the relation between the pair of operators (D, X) in $\mathsf{L}^2(\mathbb{R})$ and the pair (B, A) in $\mathsf{L}^2(\mathbb{R}_+)$ is well known and corresponds to the Mellin transform. Indeed, let $\mathscr{V} : \mathsf{L}^2(\mathbb{R}_+) \to \mathsf{L}^2(\mathbb{R})$ be defined by $(\mathscr{V} f)(x) := \mathrm{e}^{x/2} f(\mathrm{e}^x)$ for $x \in \mathbb{R}$, and remark that $\mathscr{V}$ is a unitary map with adjoint $\mathscr{V}^*$ given by $(\mathscr{V}^* g)(\lambda) = \lambda^{-1/2} g(\ln \lambda)$ for $\lambda \in \mathbb{R}_+$. Then, the Mellin transform $\mathscr{M} : \mathsf{L}^2(\mathbb{R}_+) \to \mathsf{L}^2(\mathbb{R})$ is defined by $\mathscr{M} := \mathscr{F}\mathscr{V}$ with $\mathscr{F}$ the usual unitary Fourier transform[5] in $\mathsf{L}^2(\mathbb{R})$. The main property of $\mathscr{M}$ is that it diagonalizes the generator of dilations, namely, $\mathscr{M} A \mathscr{M}^* = X$. Note that one also has $\mathscr{M} B \mathscr{M}^* = D$.

Before introducing a first isomorphic algebra, observe that if $\eta \in C([-\infty,+\infty])$, then

$$\mathscr{M}^* \eta(D) \mathscr{M} = \eta(\mathscr{M}^* D \mathscr{M}) = \eta(B) = \eta\big(-\ln(L)\big) \equiv \psi(L)$$

for some $\psi \in C([0, +\infty])$. Thus, by taking these equalities into account, it is natural to define in $\mathcal{B}\big(\mathsf{L}^2(\mathbb{R}_+)\big)$ the C^*-algebra

$$\mathcal{E}_{(L,A)} := C^*\Big(\psi_i(L)\eta_i(A) \mid \psi_i \in C([0, +\infty]) \text{ and } \eta_i \in C([-\infty, +\infty])\Big),$$

and clearly this algebra is isomorphic to the C^*-algebra $\mathcal{E}_{(D,X)}$ in $\mathcal{B}\big(\mathsf{L}^2(\mathbb{R})\big)$. Thus, through this isomorphism one gets again a short exact sequence

$$0 \to \mathcal{K}\big(\mathsf{L}^2(\mathbb{R}_+)\big) \hookrightarrow \mathcal{E}_{(L,A)} \xrightarrow{q} C(\square) \to 0$$

with the square $\square$ made of the four parts $\square = B_1 \cup B_2 \cup B_3 \cup B_4$ with $B_1 = \{0\} \times [-\infty, +\infty]$, $B_2 = [0, +\infty] \times \{+\infty\}$, $B_3 = \{+\infty\} \times [-\infty, +\infty]$, and $B_4 = [0, +\infty] \times \{-\infty\}$. In addition, the algebra $C(\square)$ of continuous functions on $\square$ can be viewed as a subalgebra of

$$C\big([-\infty, +\infty]\big) \oplus C\big([0, +\infty]\big) \oplus C\big([-\infty, +\infty]\big) \oplus C\big([0, +\infty]\big) \tag{4.7}$$

---

[5] For $f \in C_{\mathrm{c}}(\mathbb{R})$ and $x \in \mathbb{R}$ we set $[\mathscr{F} f](x) = (2\pi)^{-1/2} \int_{\mathbb{R}} \mathrm{e}^{-ixy} f(y) \, \mathrm{d}y$.

given by elements $\Gamma := (\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4)$ which coincide at the corresponding end points, that is, $\Gamma_1(+\infty) = \Gamma_2(0)$, $\Gamma_2(+\infty) = \Gamma_3(+\infty)$, $\Gamma_3(-\infty) = \Gamma_4(+\infty)$, and $\Gamma_4(0) = \Gamma_1(-\infty)$.

Finally, if one sets $\mathscr{F}_{\mathrm{s}}$ for the unitary Fourier sine transformation in $\mathsf{L}^2(\mathbb{R}_+)$, as recalled in (9.1), then the equalities $-A = \mathscr{F}_{\mathrm{s}}^* A \mathscr{F}_{\mathrm{s}}$ and $\sqrt{H_{\mathrm{D}}} = \mathscr{F}_{\mathrm{s}}^* L \mathscr{F}_{\mathrm{s}}$ hold, where H_{D} corresponds to the Dirichlet Laplacian on $\mathbb{R}_+$ introduced in Section 2. As a consequence, note that the formal equality $[i\frac{1}{2}\ln(H_{\mathrm{D}}), A] = 1$ can also be fully justified. Moreover, by using this new unitary transformation one gets that the C^*-subalgebra of $\mathcal{B}\big(\mathsf{L}^2(\mathbb{R}_+)\big)$ defined by

$$\mathcal{E}_{(H_{\mathrm{D}},A)} := C^*\Big(\psi_i(H_{\mathrm{D}})\eta_i(A) \mid \psi_i \in C([0,+\infty]) \text{ and } \varphi_i \in C([-\infty,+\infty])\Big), \quad (4.8)$$

is again isomorphic to $\mathcal{E}_{(D,X)}$, and that the quotient $\mathcal{E}_{(H_{\mathrm{D}},A)}/\mathcal{K}\big(\mathsf{L}^2(\mathbb{R}_+)\big)$ can naturally be viewed as a subalgebra of the algebra introduced in (4.7) with similar compatibility conditions. Let us mention that if the Fourier cosine transformation $\mathscr{F}_{\mathrm{c}}$ had been chosen instead of $\mathscr{F}_{\mathrm{s}}$ (see (9.2) for the definition of $\mathscr{F}_{\mathrm{c}}$) an isomorphic algebra $\mathcal{E}_{(H_{\mathrm{N}},A)}$ would have been obtained, with H_{N} the Neumann Laplacian on $\mathbb{R}_+$.

Remark 4.5. Let us stress that the presence of some minus signs in the above expressions, as for example in $B = -\ln(L)$ or in $-A = \mathscr{F}_{\mathrm{s}}^* A \mathscr{F}_{\mathrm{s}}$, are completely harmless and unavoidable. However, one can not simply forget them because they play a (minor) role in the conventions related to the computation of the winding number.

4.5. Back to the baby model

Let us briefly explain how the previous framework can be used in the context of the baby model. This will also allow us to compute explicitly the value of n in Theorem 4.4.

We consider the Hilbert space $\mathsf{L}^2(\mathbb{R}_+)$ and the unital C^*-algebra $\mathcal{E}_{(H_{\mathrm{D}},A)}$ introduced in (4.8). Let us first observe that the wave operator W_-^α of (2.2) is an isometry which clearly belongs to the C^*-algebra $\mathcal{E}_{(H_{\mathrm{D}},A)} \subset \mathcal{B}\big(\mathsf{L}^2(\mathbb{R}_+)\big)$. In addition, the image of W_-^α in the quotient algebra $\mathcal{E}_{(H_{\mathrm{D}},A)}/\mathcal{K}\big(\mathsf{L}^2(\mathbb{R}_+)\big) \cong C(\square)$ is precisely the function $\Gamma_\square^\alpha$, defined in (2.4) for $\alpha \neq 0$ and in (2.5) for $\alpha = 0$, which are unitary elements of $C(\square)$. Finally, since $C(\square)$ and $C(\mathbb{S})$ are clearly isomorphic, the winding number $\mathrm{Wind}(\Gamma_\square^\alpha)$ of $\Gamma_\square^\alpha$ can be computed, and in fact this has been performed and recorded in the table of Section 2.

On the other hand, it follows from (3.1) that $1 - (W_-^\alpha)^* W_-^\alpha = 0$ and that $1 - W_-^\alpha (W_-^\alpha)^* = E_p(H^\alpha)$, which is trivial if $\alpha \geq 0$ and which is a projection of dimension 1 if $\alpha < 0$. It follows that

$$\mathrm{Tr}\big([1 - (W_-^\alpha)^* W_-^\alpha] - [1 - W_-^\alpha (W_-^\alpha)^*]\big) = -\mathrm{Tr}\big(E_p(H^\alpha)\big) = \begin{cases} -1 & \text{if } \alpha < 0, \\ 0 & \text{if } \alpha \geq 0. \end{cases} \quad (4.9)$$

Thus, this example fits in the framework of Theorem 4.4, and in addition both sides of (4.4) have been computed explicitly. By comparing (4.9) with the results obtained for $\mathrm{Wind}(\Gamma^\alpha_\square)$, one gets that the factor n mentioned in (4.4) is equal to -1 for these algebras. Finally, since $E_p(H^\alpha)$ is related to the point spectrum of H^α, the content of Proposition 2.2 can be rewritten as

$$\mathrm{Wind}(\Gamma^\alpha_\square) = \sharp\sigma_{\mathrm{p}}(H^\alpha).$$

This equality corresponds to a topological version of Levinson's theorem for the baby model. Obviously, this result was already obtained in Section 2 and all the above framework was not necessary for its derivation. However, we have now in our hands a very robust framework which will be applied to several other situations.

5. Quasi 1D examples

In this section, we gather various examples of scattering systems which can be recast in the framework introduced in the previous section. Several topological versions of Levinson's theorem will be deduced for these models. Note that we shall avoid in this section the technicalities required for obtaining more explicit formulas for the wave operators. An example of such a rather detailed proof will be provided for Schrödinger operators on $\mathbb{R}^3$.

5.1. Schrödinger operator with one point interaction

In this section we recall the results which have been obtained for Schrödinger operators with one point interaction. In fact, such operators were the first ones on which the algebraic framework has been applied. More information about this model can be found in [30]. Note that the construction and the results depend on the space dimension, we shall therefore present successively the results in dimension 1, 2 and 3. However, even in dimension 2 and 3, the problem is essentially one-dimensional, as we shall observe.

Let us consider the Hilbert space $\mathsf{L}^2(\mathbb{R}^d)$ and the operator $H_0 = -\Delta$ with domain the Sobolev space $\mathcal{H}^2(\mathbb{R}^d)$. For the operator H we shall consider the perturbation of H_0 by a one point interaction located at the origin of $\mathbb{R}^d$. We shall not recall the precise definition of a one point interaction since this subject is rather well known, and since the literature on the subject is easily accessible. Let us just mention that such a perturbation of H_0 corresponds to the addition of a boundary condition at $0 \in \mathbb{R}^d$ which can be parameterized by a single real parameter family in $\mathbb{R}^d$ for $d = 2$ and $d = 3$. In dimension 1 a four real parameters family is necessary for describing all corresponding operators. In the sequel and in dimension 1 we shall deal only with either a so-called δ-interaction or a δ'-interaction. We refer for example to the monograph [2] for a thorough presentation of operators with a finite or an infinite number of point interactions.

Beside the action of dilations in $\mathsf{L}^2(\mathbb{R}_+)$, we shall often use the dilation groups in $\mathsf{L}^2(\mathbb{R}^d)$ whose action is defined by

$$[U_t f](x) = \mathrm{e}^{dt/2} f\big(\mathrm{e}^t x\big), \qquad f \in \mathsf{L}^2(\mathbb{R}^d),\ x \in \mathbb{R}^d.$$

Generically, its generator will be denoted by A in all these spaces.

5.1.1. The dimension $d = 1$. For any $\alpha, \beta \in \mathbb{R}$, let us denote by H^α the operator in $\mathsf{L}^2(\mathbb{R})$ which formally corresponds to $H_0 + \alpha\delta$ and by H^β the operator which formally corresponds to $H_0 + \beta\delta'$. Note that for $\alpha < 0$ and for $\beta < 0$ the operators H^α and H^β have both a single eigenvalue of multiplicity one, while for $\alpha \geq 0$ and for $\beta \geq 0$ the corresponding operators have no eigenvalue. It is also known that the wave operators $W_\pm^\alpha$ for the pair (H^α, H_0) exist, and that the wave operators $W_\pm^\beta$ for the pair (H^β, H_0) also exist. Some explicit expressions for them have been computed in [30].

Lemma 5.1. *For any $\alpha, \beta \in \mathbb{R}$ the following equalities hold in $\mathcal{B}\big(\mathsf{L}^2(\mathbb{R})\big)$:*

$$W_-^\alpha = 1 + \tfrac{1}{2}\big(1 + \tanh(\pi A) + i\cosh(\pi A)^{-1}\big)\Big[\frac{2\sqrt{H_0} - i\alpha}{2\sqrt{H_0} + i\alpha} - 1\Big]P_{\mathrm{e}},$$

$$W_-^\beta = 1 + \tfrac{1}{2}\big(1 + \tanh(\pi A) - i\cosh(\pi A)^{-1}\big)\Big[\frac{2 + i\beta\sqrt{H_0}}{2 - i\beta\sqrt{H_0}} - 1\Big]P_{\mathrm{o}},$$

where P_{e} denotes the projection onto the set of even functions of $\mathsf{L}^2(\mathbb{R})$, while P_{o} denotes the projection onto the set of odd functions of $\mathsf{L}^2(\mathbb{R})$.

In order to come back precisely to the framework introduced in Section 4, we need to introduce the even / odd representation of $\mathsf{L}^2(\mathbb{R})$. Given any function m on $\mathbb{R}$, we write m_{e} and m_{o} for the even part and the odd part of m. We also set $\mathscr{H} := \mathsf{L}^2(\mathbb{R}_+; \mathbb{C}^2)$ and introduce the unitary map $\mathscr{U} : \mathsf{L}^2(\mathbb{R}) \to \mathscr{H}$ given on any $f \in \mathsf{L}^2(\mathbb{R})$, $\big(\begin{smallmatrix} f_1 \\ f_2 \end{smallmatrix}\big) \in \mathscr{H}$, $x \in \mathbb{R}$ by

$$\mathscr{U} f := \sqrt{2}\begin{pmatrix} f_{\mathrm{e}} \\ f_{\mathrm{o}} \end{pmatrix} \quad \text{and} \quad \big[\mathscr{U}^*\big(\begin{smallmatrix} f_1 \\ f_2 \end{smallmatrix}\big)\big](x) := \tfrac{1}{\sqrt{2}}[f_1(|x|) + \mathrm{sgn}(x) f_2(|x|)]. \tag{5.1}$$

Now, observe that if m is a function on $\mathbb{R}$ and $m(X)$ denotes the corresponding multiplication operator on $\mathsf{L}^2(\mathbb{R})$, then we have

$$\mathscr{U} m(X) \mathscr{U}^* = \begin{pmatrix} m_{\mathrm{e}}(L) & m_{\mathrm{o}}(L) \\ m_{\mathrm{o}}(L) & m_{\mathrm{e}}(L) \end{pmatrix}$$

where L is the operator of multiplication by the variable in $\mathsf{L}^2(\mathbb{R}_+)$ already introduced in (4.6).

By taking these formulas and the previous lemma into account, one gets

$$\mathscr{U} W_-^\alpha \mathscr{U}^* = \begin{pmatrix} 1 + \frac{1}{2}\big(1 + \tanh(\pi A) + i\cosh(\pi A)^{-1}\big)\Big[\frac{2\sqrt{H_{\mathrm{N}}} - i\alpha}{2\sqrt{H_{\mathrm{N}}} + i\alpha} - 1\Big] & 0 \\ 0 & 1 \end{pmatrix}$$

$$\mathscr{U} W_-^\beta \mathscr{U}^* = \begin{pmatrix} 1 & 0 \\ 0 & 1 + \frac{1}{2}\big(1 + \tanh(\pi A) - i\cosh(\pi A)^{-1}\big)\Big[\frac{2 + i\beta\sqrt{H_{\mathrm{D}}}}{2 - i\beta\sqrt{H_{\mathrm{D}}}} - 1\Big] \end{pmatrix}$$

It clearly follows from these formulas that

$$\mathscr{U} W_-^\alpha \mathscr{U}^* \in \mathcal{M}_2\big(\mathcal{E}_{(H_{\mathrm{N}}, A)}\big) \quad \text{and} \quad \mathscr{U} W_-^\beta \mathscr{U}^* \in \mathcal{M}_2\big(\mathcal{E}_{(H_{\mathrm{D}}, A)}\big),$$

and as a consequence the algebraic framework introduced in Section 4 can be applied straightforwardly. In particular, one can define the functions $\Gamma_\square^\alpha$, $\Gamma_\square^\beta$ as the image of $\mathscr{U} W_-^\alpha \mathscr{U}^*$ and $\mathscr{U} W_-^\beta \mathscr{U}^*$ in the respective quotient algebras, and get:

Corollary 5.2. *For any $\alpha, \beta \in \mathbb{R}^*$, one has*

$$\Gamma^\alpha_\square = \left(\begin{pmatrix} 1+\frac{1}{2}(1+\tanh(\pi\cdot)+i\cosh(\pi\cdot)^{-1})[s^\alpha(0)-1] & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} s^\alpha(\cdot) & 0 \\ 0 & 1 \end{pmatrix}, \right.$$
$$\left. \begin{pmatrix} 1+\frac{1}{2}(1+\tanh(\pi\cdot)+i\cosh(\pi\cdot)^{-1})[s^\alpha(+\infty)-1] & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right)$$

with $s^\alpha(\cdot) = \frac{2\sqrt{\cdot}-i\alpha}{2\sqrt{\cdot}+i\alpha}$,

$$\Gamma^\beta_\square = \left(\begin{pmatrix} 1 & 0 \\ 0 & 1+\frac{1}{2}(1+\tanh(\pi\cdot)-i\cosh(\pi\cdot)^{-1})[s^\beta(0)-1] \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & s^\beta(\cdot) \end{pmatrix}, \right.$$
$$\left. \begin{pmatrix} 1 & 0 \\ 0 & 1+\frac{1}{2}(1+\tanh(\pi\cdot)-i\cosh(\pi\cdot)^{-1})[s^\beta(+\infty)-1] \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right)$$

with $s^\beta(\cdot) = \frac{2+i\beta\sqrt{\cdot}}{2-i\beta\sqrt{\cdot}}$, *and* $\Gamma^0_\square = (1_2, 1_2, 1_2, 1_2)$ (*both for* $\alpha = 0$ *and* $\beta = 0$). *In addition, one infers that for any $\alpha, \beta \in \mathbb{R}$:*

$$\mathrm{Wind}(\Gamma^\alpha_\square) = \sharp\sigma_{\mathrm{p}}(H^\alpha), \qquad \textit{and} \qquad \mathrm{Wind}(\Gamma^\beta_\square) = \sharp\sigma_{\mathrm{p}}(H^\beta).$$

Remark 5.3. Let us mention that another convention had been taken in [30] for the computation of the winding number, leading to a different sign in the previous equalities. Note that the same remark holds for equations (5.3) and (5.5) below.

5.1.2. The dimension $d = 2$. As already mentioned above, in dimension 2 there is only one type of self-adjoint extensions, and thus only one real parameter family of operators H^α which formally correspond to $H_0 + \alpha\delta$. The main difference with dimensions 1 and 3 is that H^α always possesses a single eigenvalue of multiplicity one. As before, the wave operators $W^\alpha_\pm$ for the pair (H^α, H_0) exist, and it has been shown in the reference paper that:

Lemma 5.4. *For any $\alpha \in \mathbb{R}$ the following equality holds:*

$$W^\alpha_- = 1 + \tfrac{1}{2}\big(1+\tanh(\pi A/2)\big)\left[\frac{2\pi\alpha - \Psi(1) - \ln(2) + \ln(\sqrt{H_0}) + i\pi/2}{2\pi\alpha - \Psi(1) - \ln(2) + \ln(\sqrt{H_0}) - i\pi/2} - 1\right] P_0,$$

where P_0 denotes the projection on the spherically symmetric functions of $\mathsf{L}^2(\mathbb{R}^2)$, and where Ψ corresponds to the digamma function.

Note that in this formula, A denotes the generator of dilations in $\mathsf{L}^2(\mathbb{R}^2)$. It is then sufficient to restrict our attention to $P_0\mathsf{L}^2(\mathbb{R}^2)$ since the subspace of $\mathsf{L}^2(\mathbb{R}^2)$ which is orthogonal to $P_0\mathsf{L}^2(\mathbb{R}^2)$ does not play any role for this model (and it is the reason why this model is quasi one-dimensional). Thus, let us introduce the unitary map $\mathscr{U} : P_0\mathsf{L}^2(\mathbb{R}^2) \to \mathsf{L}^2(\mathbb{R}_+, r\mathrm{d}r)$ defined by $[\mathscr{U} f](r) := \sqrt{2\pi} f(r)$ which is well defined since $f \in P_0\mathsf{L}^2(\mathbb{R}^2)$ depends only on the radial coordinate. Since the dilation group as well as the operator H_0 leave the subspace $P_0\mathsf{L}^2(\mathbb{R}^2)$ of $\mathsf{L}^2(\mathbb{R}^2)$ invariant, one gets in $\mathsf{L}^2(\mathbb{R}_+, r\mathrm{d}r)$:

$$\mathscr{U} W^\alpha_- P_0 \mathscr{U}^* = 1 + \tfrac{1}{2}\big(1+\tanh(\pi A/2)\big)\left[\frac{2\pi\alpha - \Psi(1) - \ln(2) + \ln(\sqrt{H_0}) + i\pi/2}{2\pi\alpha - \Psi(1) - \ln(2) + \ln(\sqrt{H_0}) - i\pi/2} - 1\right]. \tag{5.2}$$

Remark 5.5. Let us stress that the above formula does not take place in any of the representations introduced in Section 4.4 but in a unitarily equivalent one. Indeed, one can come back to the algebra $\mathcal{E}_{(L,A)}$ by using the spectral representation of H_0. More precisely let us first introduce $\mathscr{F}_0 : \mathsf{L}^2(\mathbb{R}^2) \to \mathsf{L}^2\big(\mathbb{R}_+; \mathsf{L}^2(\mathbb{S})\big)$ defined by

$$\big([\mathscr{F}_0 f](\lambda)\big)(\omega) = 2^{-1/2}[\mathscr{F} f](\sqrt{\lambda}\omega), \qquad f \in C_c(\mathbb{R}^2),\ \lambda \in \mathbb{R}_+,\ \omega \in \mathbb{S}$$

with $\mathscr{F}$ the unitary Fourier transform in $\mathsf{L}^2(\mathbb{R}^2)$, and recall that $[\mathscr{F}_0 H_0 f](\lambda) = \lambda[\mathscr{F}_0 f](\lambda)$ for any $f \in \mathcal{H}^2(\mathbb{R}^2)$ and a.e. $\lambda \in \mathbb{R}_+$. Then, if one defines the unitary map $\mathscr{U}' : P_0\mathsf{L}^2(\mathbb{R}^2) \to \mathsf{L}^2(\mathbb{R}_+)$ by $[\mathscr{U}' f](\lambda) := \sqrt{\pi}[\mathscr{F} f](\sqrt{\lambda})$, one gets $\mathscr{U}' H_0 \mathscr{U}'^* = L$, and a short computation using the dilation group in $\mathsf{L}^2(\mathbb{R}^2)$ and in $\mathsf{L}^2(\mathbb{R}_+)$ leads to the relation $\mathscr{U}' A \mathscr{U}'^* = -2A$. As a consequence of this alternative construction, the following equality holds in $\mathsf{L}^2(\mathbb{R}_+)$:

$$\mathscr{U}' W_-^\alpha P_0 \mathscr{U}'^* = 1 + \tfrac{1}{2}\big(1 - \tanh(\pi A)\big)\left[\frac{2\pi\alpha - \Psi(1) - \ln(2) + \ln(\sqrt{L}) + i\pi/2}{2\pi\alpha - \Psi(1) - \ln(2) + \ln(\sqrt{L}) - i\pi/2} - 1\right]$$

and it is then clear that this operator belongs to $\mathcal{E}_{(L,A)}$.

By coming back to the expression (5.2) one can compute the image $\Gamma_\square^\alpha$ of this operator in the quotient algebra and obtain the following statement:

Corollary 5.6. *For any $\alpha \in \mathbb{R}$, one has $\Gamma_\square^\alpha = \big(1, s^\alpha(\cdot), 1, 1\big)$ and*

$$\mathrm{Wind}(\Gamma_\square^\alpha) = \mathrm{Wind}(s^\alpha) = \sharp\sigma_{\mathrm{p}}(H^\alpha) = 1, \tag{5.3}$$

with $s^\alpha(\cdot) = \frac{2\pi\alpha - \Psi(1) - \ln(2) + \ln(\sqrt{\cdot}) + i\pi/2}{2\pi\alpha - \Psi(1) - \ln(2) + \ln(\sqrt{\cdot}) - i\pi/2}$.

5.1.3. The dimension $d = 3$. In dimension 3, there also exists only one real parameter family of self-adjoint operators H^α formally represented as $H_0 + \alpha\delta$, and this operator has a single eigenvalue if $\alpha < 0$ and no eigenvalue if $\alpha \geq 0$. As for the other two dimensions, the wave operators $W_\pm^\alpha$ for the pair (H^α, H_0) exist, and it has been shown in the reference paper that:

Lemma 5.7. *For any $\alpha \in \mathbb{R}$ the following equality holds*

$$W_-^\alpha = 1 + \tfrac{1}{2}\big(1 + \tanh(\pi A) - i\cosh(\pi A)^{-1}\big)\left[\frac{4\pi\alpha + i\sqrt{H_0}}{4\pi\alpha - i\sqrt{H_0}} - 1\right] P_0\ .$$

where P_0 denotes the projection on the spherically symmetric functions of $\mathsf{L}^2(\mathbb{R}^3)$.

Note that in these formulas, A denotes the generator of dilations in $\mathsf{L}^2(\mathbb{R}^3)$. As for the two-dimensional case, it is sufficient to restrict our attention to $P_0\mathsf{L}^2(\mathbb{R}^3)$ since the subspace of $\mathsf{L}^2(\mathbb{R}^3)$ which is orthogonal to $P_0\mathsf{L}^2(\mathbb{R}^3)$ does not play any role for this model (and it is again the reason why this model is quasi one-dimensional). Let us thus introduce the unitary map $\mathscr{U} : P_0\mathsf{L}^2(\mathbb{R}^3) \to \mathsf{L}^2(\mathbb{R}_+, r^2\mathrm{d}r)$ defined by $[\mathscr{U} f](r) := 2\sqrt{\pi} f(r)$ which is well defined since $f \in P_0\mathsf{L}^2(\mathbb{R}^3)$ depends only on the radial coordinate. Since the dilation group as well as the operator H_0 leave the subspace $P_0\mathsf{L}^2(\mathbb{R}^3)$ of $\mathsf{L}^2(\mathbb{R}^3)$ invariant, one gets in $\mathsf{L}^2(\mathbb{R}_+, r^2\mathrm{d}r)$:

$$\mathscr{U} W_-^\alpha P_0 \mathscr{U}^* = 1 + \tfrac{1}{2}\big(1+\tanh(\pi A) - i\cosh(\pi A)^{-1}\big)\left[\frac{4\pi\alpha + i\sqrt{H_0}}{4\pi\alpha - i\sqrt{H_0}} - 1\right]. \quad (5.4)$$

Remark 5.8. As in the two-dimensional case, the above formula does not take place in any of the representations introduced in Section 4.4 but in a unitarily equivalent one. In this case again, one can come back to the algebra $\mathcal{E}_{(L,A)}$ by using the spectral representation of H_0. We refer to the 2-dimensional case for the details.

By coming back to the expression (5.4) one can compute the image $\Gamma_\square^\alpha$ of this operator in the quotient algebra. If one sets $s^\alpha(\cdot) = \frac{4\pi\alpha + i\sqrt{\cdot}}{4\pi\alpha - i\sqrt{\cdot}}$ one gets:

Corollary 5.9. *For any $\alpha \in \mathbb{R}^*$, one has*

$$\Gamma_\square^\alpha = \big(1, s^\alpha(\cdot), -\tanh(\pi\cdot) + i\cosh(\pi\cdot)^{-1}, 1\big)$$

while $\Gamma_\square^0 = \big(-\tanh(\pi\cdot) + i\cosh(\pi\cdot)^{-1}, -1, -\tanh(\pi\cdot) + i\cosh(\pi\cdot)^{-1}, 1\big)$. *In addition, for any $\alpha \in \mathbb{R}$ it follows that*

$$\mathrm{Wind}(\Gamma_\square^\alpha) = \sharp\sigma_{\mathrm{p}}(H^\alpha). \quad (5.5)$$

As before, we refer to [30] for the details of the computations, but stress that some conventions had been chosen differently.

5.2. Schrödinger operator on $\mathbb{R}$

The content of this section is mainly borrowed from [31] but some minor adaptations with respect to this paper are freely made. We refer to this reference and to the papers mentioned in it for more information on scattering theory for Schrödinger operators on $\mathbb{R}$.

We consider the Hilbert space $\mathsf{L}^2(\mathbb{R})$, and the self-adjoint operators $H_0 = -\Delta$ with domain $\mathcal{H}^2(\mathbb{R})$ and $H = H_0 + V$ with V a multiplication operator by a real function which satisfies the condition

$$\int_{\mathbb{R}} (1+|x|)^\rho |V(x)|\,\mathrm{d}x < \infty, \quad (5.6)$$

for some $\rho \geq 1$. For such a pair of operators, it is well known that the conditions required by Assumption 3.1 are satisfied, and thus that the wave operators $W_\pm$ are Fredholm operators and the scattering operator S is unitary.

In order to use the algebraic framework introduced in Section 4, more information on the wave operators are necessary. First of all, let us recall the following statement which has been proved in [31].

Proposition 5.10. *Assume that V satisfies* (5.6) *with $\rho > 5/2$, then the following representation of the wave operator holds:*

$$W_- = 1 + \tfrac{1}{2}\big(1+\tanh(\pi A) + i\cosh(\pi A)^{-1}(P_{\mathrm{e}} - P_{\mathrm{o}})\big)[S-1] + K$$

with K a compact operator in $\mathsf{L}^2(\mathbb{R})$, and $P_{\mathrm{e}}, P_{\mathrm{o}}$ the projections on the even elements, respectively odd elements, of $\mathsf{L}^2(\mathbb{R})$.

Let us now look at this result in the even / odd representation introduced in Section 5.1.1. More precisely, by using the map $\mathscr{U} : \mathsf{L}^2(\mathbb{R}) \to \mathsf{L}^2(\mathbb{R}_+;\mathbb{C}^2)$ introduced in (5.1), one gets

$$\begin{aligned}&\mathscr{U} W_- \mathscr{U}^* \qquad (5.7)\\ &= 1_2 + \tfrac{1}{2}\begin{pmatrix} 1+\tanh(\pi A)+i\cosh(\pi A)^{-1} & 0 \\ 0 & 1+\tanh(\pi A)-i\cosh(\pi A)^{-1}\end{pmatrix}\Big[S\begin{pmatrix} H_{\mathrm{N}} & 0 \\ 0 & H_{\mathrm{D}}\end{pmatrix} - 1_2\Big] + K'\end{aligned}$$

with $K' \in \mathcal{K}\big(\mathsf{L}^2(\mathbb{R}_+;\mathbb{C}^2)\big)$.

Remark 5.11. As in the previous example, the operator $\mathscr{U} W_- \mathscr{U}^*$ does not belong directly to one of the algebras introduced in Section 4.4, but in a unitarily equivalent one which can be constructed with the spectral representation of H_0. More precisely, we set $\mathscr{F}_0 : \mathsf{L}^2(\mathbb{R}) \to \mathsf{L}^2(\mathbb{R}_+;\mathbb{C}^2)$ defined by

$$[\mathscr{F}_0 f](\lambda) = 2^{-1/2}\lambda^{-1/4}\begin{pmatrix}[\mathscr{F} f](-\sqrt{\lambda}) \\ [\mathscr{F} f](\sqrt{\lambda})\end{pmatrix} \qquad f \in C_{\mathrm{c}}(\mathbb{R}),\ \lambda \in \mathbb{R}_+$$

with $\mathscr{F}$ the unitary Fourier transform in $\mathsf{L}^2(\mathbb{R})$. As usual, one has $[\mathscr{F}_0 H_0 f](\lambda) = \lambda[\mathscr{F}_0 f](\lambda)$ for any $f \in \mathcal{H}^2(\mathbb{R})$ and a.e. $\lambda \in \mathbb{R}_+$. Accordingly, one writes $L \otimes 1_2 = \mathscr{F}_0 H_0 \mathscr{F}_0^*$. Similarly, the equality $\mathscr{F}_0 A \mathscr{F}_0^* = -2A \otimes 1_2$ holds, where the operator A on the l.h.s. corresponds to the generator of dilation in $\mathsf{L}^2(\mathbb{R})$, while the operator A on the r.h.s. corresponds to the generator of dilations in $\mathsf{L}^2(\mathbb{R}_+)$. Finally, a short computation leads to the equalities $\mathscr{F}_0 P_{\mathrm{e}} \mathscr{F}_0^* = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1\end{pmatrix}$ and $\mathscr{F}_0 P_{\mathrm{o}} \mathscr{F}_0^* = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1\end{pmatrix}$. By summing up these information one gets

$$\mathscr{F}_0 W_- \mathscr{F}_0^* = 1_2 + \tfrac{1}{2}\begin{pmatrix} 1-\tanh(2\pi A) & i\cosh(2\pi A)^{-1} \\ i\cosh(2\pi A)^{-1} & 1-\tanh(2\pi A)\end{pmatrix}\big[S(L) - 1_2\big] + \mathscr{F}_0 K \mathscr{F}_0^* \ . \qquad (5.8)$$

Based on this formula, it is clear that $\mathscr{F}_0 W_- \mathscr{F}_0^*$ belongs to $\mathcal{M}_2(\mathcal{E}_{(L,A)})$, as it should be.

Let us however come back to formula (5.7) and compute the image $\Gamma_\square$ of this operator in the quotient algebra. One clearly gets

$$\Gamma_\square = \Big(1_2 + \tfrac{1}{2}\begin{pmatrix} 1+\tanh(\pi\cdot)+i\cosh(\pi\cdot)^{-1} & 0 \\ 0 & 1+\tanh(\pi\cdot)-i\cosh(\pi\cdot)^{-1}\end{pmatrix}[S(0)-1_2], S(\cdot), 1_2, 1_2\Big). \qquad (5.9)$$

In addition, let us note that under our condition on V, the map $\mathbb{R}_+ \ni \lambda \mapsto S(\lambda) \in \mathcal{M}_2(\mathbb{C})$ is norm continuous and has a limit at 0 and converges to 1_2 at $+\infty$. Then, by the algebraic formalism, one would automatically obtain that the winding number of the pointwise determinant of the function $\Gamma_\square$ is equal to the number of bound states of H. However, let us add some more comments on this model, and in particular on the matrix $S(0)$. In fact, it is well known that the matrix $S(0)$ depends on the existence or the absence of a so-called half-bound state for H at 0. Before explaining this statement, let us recall a result which has been proved in [31, Prop. 9], and which is based only on the explicit expression (5.9) and its unitarity.

Lemma 5.12. *Either* $\det\big(S(0)\big) = -1$ *and then* $S(0) = \pm\left(\begin{smallmatrix} -1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$, *or* $\det\big(S(0)\big) = 1$ *and then* $S(0) = \left(\begin{smallmatrix} a & b \\ -\bar{b} & a \end{smallmatrix}\right)$ *with* $a \in \mathbb{R}$, $b \in \mathbb{C}$ *and* $|a|^2 + |b|^2 = 1$. *Moreover, the contribution to the winding number of the first term of* $\Gamma_\square$ *is equal to* $\pm\frac{1}{2}$ *in the first case, and to* 0 *in the second case.*

Let us now mention that when H possesses a half-bound state, *i.e.*, a solution of the equation $Hf = 0$ with f in $\mathsf{L}^\infty(\mathbb{R})$ but not in $\mathsf{L}^2(\mathbb{R})$, then $\det\big(S(0)\big) = 1$. This case is called the exceptional case, and thus the first term in $\Gamma_\square$ does not provide any contribution to the winding number in this case. On the other hand, when H does not possess such a half-bound state, then $S(0) = \left(\begin{smallmatrix} -1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$. This case is referred as the generic case, and in this situation the first term in $\Gamma_\square$ provides a contribution of $\frac{1}{2}$ to the winding number. By taking these information into account, Levinson's theorem can be rewritten for this model as

$$\mathrm{Wind}(S) = \begin{cases} \sharp\sigma_{\mathrm{p}}(H) - \frac{1}{2} & \text{in the generic case,} \\ \sharp\sigma_{\mathrm{p}}(H) & \text{in the exceptional case.} \end{cases}$$

Such a result is in accordance with the classical literature on the subject, see [31] and references therein for the proof of the above statements and for more explanations. Note finally that one asset of our approach has been to show that the correction $-\frac{1}{2}$ should be located on the other side of the above equality (with a different sign), and that the rearranged equality is in fact an index theorem.

5.3. Rank one interaction

In this section, we present another scattering system which has been studied in [46]. Our interest in this model comes from the spectrum of H_0 which is equal to $\mathbb{R}$. This fact implies in particular that if H possesses some eigenvalues, then these eigenvalues are automatically included in the spectrum of H_0. In our approach, this fact does not cause any problem, but some controversies for the original Levinson theorem with embedded eigenvalues can be found in the literature, see [15]. Note that the following presentation is reduced to the key features only, all the details can be found in the original paper.

We consider the Hilbert space $\mathsf{L}^2(\mathbb{R})$, and let H_0 be the operator of multiplication by the variable, *i.e.*, $H_0 = X$, as introduced at the beginning of Section 4.4. For the perturbation, let $u \in \mathsf{L}^2(\mathbb{R})$ and consider the rank one perturbation of H_0 defined by

$$H_u f = H_0 f + \langle u, f\rangle u, \qquad f \in \mathcal{D}(H_0).$$

It is well known that for such a rank one perturbation the wave operators exist and that the scattering operator is unitary. Note that for this model, the scattering operator $S \equiv S(X)$ is simply an operator of multiplication by a function defined on $\mathbb{R}$ and taking values in $\mathbb{T}$. Let us also stress that for such a general u singular continuous spectrum for H can exist. In order to ensure the asymptotic completeness, an additional condition on u is necessary. More precisely, let us introduce this additional assumption:

Assumption 5.13. *The function* $u \in \mathsf{L}^2(\mathbb{R})$ *is Hölder continuous with exponent* $\alpha > 1/2$.

It is known that under Assumption 5.13, the operator H_u has at most a finite number of eigenvalues of multiplicity one [3, Sec. 2]. In addition, it is proved in [46, Lem. 2.2] that under this assumption the map

$$S : \mathbb{R} \ni x \mapsto S(x) \in \mathbb{T}$$

is continuous and satisfies $S(\pm\infty) = 1$.

In order to state the main result about the wave operators for this model, let us use again the even / odd representation of $\mathsf{L}^2(\mathbb{R})$ introduced in Section 5.1.1. Let us also recall that we set m_{e}, m_{o} for the even part and the odd part of any function m defined on $\mathbb{R}$.

Theorem 5.14 (Theorem 1.2 of [46]). *Let* u *satisfy Assumption* 5.13. *Then, one has*

$$\mathscr{U} W_- \mathscr{U}^* \tag{5.10}$$
$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 & -\tanh(\pi A) + i\cosh(\pi A)^{-1} \\ -\tanh(\pi A) - i\cosh(\pi A)^{-1} & 1 \end{pmatrix} \begin{pmatrix} S_{\mathrm{e}}(L)-1 & S_{\mathrm{o}}(L) \\ S_{\mathrm{o}}(L) & S_{\mathrm{e}}(L)-1 \end{pmatrix} + K,$$

where K *is a compact operator in* $\mathsf{L}^2(\mathbb{R}_+;\mathbb{C}^2)$.

Let us immediately mention that a similar formula holds for W_+ and that this formula is exhibited in the reference paper. In addition, it follows from (5.10) that $W_- \in \mathcal{M}_2\big(\mathcal{E}_{(L,A)}\big)$, and that the algebraic framework introduced in Section 4 can be applied straightforwardly. Without difficulty, the formalism leads us directly to the following consequence of Theorem 5.14:

Corollary 5.15. *Let* u *satisfy Assumption* 5.13. *Then the following equality holds:*

$$\mathrm{Wind}(S) = \sharp\sigma_{\mathrm{p}}(H_u).$$

Let us stress that another convention had been taken in [46] for the computation of the winding number, leading to a different sign in the previous equality. Note also that such a result was already known for more general perturbations but under stronger regularity conditions [10, 16]. We stress that the above result does require neither the differentiability of the scattering matrix nor the differentiability of u. It is also interesting that for this model, only the winding number of the scattering operator contributes to the left-hand side of the equality.

5.4. Other examples

In this section, we simply mention two additional models on which some investigations have been performed in relation with our topological approach of Levinson's theorem.

In reference [22], the so-called Friedrichs–Faddeev model has been studied. In this model, the operator H_0 corresponds to the multiplication by the variable but only on an interval $[a,b]$, and not on $\mathbb{R}$. The perturbation of H_0 is defined in terms of an integral operator which satisfies some Hölder continuity conditions, and some additional conditions on the restriction of the kernel at the values a and b are imposed. Explicit expressions for the wave operators for this model have been provided in [22], but the use of these formulas for deducing a topological Levinson theorem has not been performed yet. Note that one of the interests in this model is that the spectrum of H_0 is equal to $[a, b]$, which is different from $\mathbb{R}_+$ or $\mathbb{R}$ which appear in the models developed above.

In reference [42], the spectral and scattering theory for 1-dimensional Dirac operators with mass $m > 0$ and with a zero-range interaction are fully investigated. In fact, these operators are described by a four real parameters family of self-adjoint extensions of a symmetric operator. Explicit expressions for the wave operators and for the scattering operator are provided. Let us note that these new formulas take place in a representation which links, in a suitable way, the energies $-\infty$ and $+\infty$, and which emphasizes the role of the thresholds $\pm m$. Based on these formulas, a topological version of Levinson's theorem is deduced, with the threshold effects at $\pm m$ automatically taken into account. Let us also emphasize that in our investigations on Levinson's theorem, this model was the first one for which the spectrum of H_0 consisted into two disjoint parts, namely $(-\infty, -m] \cup [+m, \infty)$. It was not clear at the very beginning what could be the suitable algebra for nesting the wave operators and how the algebraic construction could then be used. The results of these investigations are thoroughly presented in [42], and it is expected that the same results hold for less singular perturbations of H_0. Finally, a surprising feature of this model is that the contribution to the winding number from the scattering matrix is computed from $-m$ to $-\infty$, and then from $+m$ to $+\infty$. In addition, contributions due to thresholds effects can appear at $-m$ and/or at $+m$.

6. Schrödinger on $\mathbb{R}^3$ and regularized Levinson theorem

In this section, we illustrate our approach on the example of a Schrödinger operator on $\mathbb{R}^3$. In the first part, we explain with some details how new formulas for the wave operators can be obtained for this model. In a second part, the algebraic framework is slightly enlarged in order to deal with a spectrum with infinite multiplicity. A method of regularization for the computation of the winding number is also presented.

6.1. New expressions for the wave operators

In this section, we derive explicit formulas for the wave operators based on the stationary approach of scattering theory. Let us immediately stress that the following presentation is deeply inspired from the paper [47] to which we refer for the proofs and for more details. Thus, our aim is to justify the following statement:

Theorem 6.1. *Let $V \in \mathsf{L}^\infty(\mathbb{R}^3)$ be real and satisfy $|V(x)| \leq \text{Const.}\,(1 + |x|)^{-\rho}$ with $\rho > 7$ for almost every $x \in \mathbb{R}^3$. Then, the wave operators $W_\pm$ for the pair of operators $(-\Delta + V, -\Delta)$ exist and the following equalities hold in $\mathcal{B}\big(\mathsf{L}^2(\mathbb{R}^3)\big)$:*

$$W_- = 1 + \tfrac{1}{2}\big(1 + \tanh(\pi A) - i\cosh(\pi A)^{-1}\big)[S - 1] + K$$

and

$$W_+ = 1 + \tfrac{1}{2}\big(1 - \tanh(\pi A) + i\cosh(\pi A)^{-1}\big)[S^* - 1] + K',$$

with A is the generator of dilations in $\mathbb{R}^3$, S the scattering operator, and $K, K' \in \mathcal{K}\big(\mathsf{L}^2(\mathbb{R}^3)\big)$.

In order to prove this statement, let us be more precise about the framework. We first introduce the Hilbert space $\mathcal{H} := \mathsf{L}^2(\mathbb{R}^3)$ and the self-adjoint operator $H_0 = -\Delta$ with domain the usual Sobolev space $\mathcal{H}^2 \equiv \mathcal{H}^2(\mathbb{R}^3)$. We also set $\mathscr{H} := \mathsf{L}^2(\mathbb{R}_+; \mathfrak{h})$ with $\mathfrak{h} := \mathsf{L}^2\big(\mathbb{S}^2\big)$, and $\mathcal{S}(\mathbb{R}^3)$ for the Schwartz space on $\mathbb{R}^3$. The spectral representation for H_0 is constructed as follows: we define $\mathscr{F}_0 : \mathsf{L}^2(\mathbb{R}^3) \to \mathsf{L}^2(\mathbb{R}_+; \mathfrak{h})$ by

$$\begin{aligned}\big([\mathscr{F}_0 f](\lambda)\big)(\omega) &= \big(\tfrac{\lambda}{4}\big)^{1/4}[\mathscr{F} f](\sqrt{\lambda}\,\omega) \\ &= \big(\tfrac{\lambda}{4}\big)^{1/4}\big[\gamma(\sqrt{\lambda})\mathscr{F} f\big](\omega), \quad f \in \mathcal{S}(\mathbb{R}^3),\ \lambda \in \mathbb{R}_+,\ \omega \in \mathbb{S}^2,\end{aligned}$$

with $\gamma(\lambda) : \mathcal{S}(\mathbb{R}^3) \to \mathfrak{h}$ the trace operator given by $\big[\gamma(\lambda) f\big](\omega) := f(\lambda\,\omega)$, and $\mathscr{F}$ the unitary Fourier transform on $\mathbb{R}^3$. The map $\mathscr{F}_0$ is unitary and satisfies for $f \in \mathcal{H}^2$ and a.e. $\lambda \in \mathbb{R}_+$

$$[\mathscr{F}_0 H_0 f](\lambda) = \lambda[\mathscr{F}_0 f](\lambda) \equiv [L\mathscr{F}_0 f](\lambda),$$

where L denotes the multiplication operator in $\mathscr{H}$ by the variable in $\mathbb{R}_+$.

Let us now introduce the operator $H := H_0 + V$ with a potential $V \in \mathsf{L}^\infty(\mathbb{R}^3; \mathbb{R})$ satisfying for some $\rho > 1$ the condition

$$|V(x)| \le \text{Const.}\,\langle x\rangle^{-\rho}, \quad \text{a.e. } x \in \mathbb{R}^3, \tag{6.1}$$

with $\langle x\rangle := \sqrt{1 + x^2}$. Since V is bounded, H is self-adjoint with domain $\mathcal{D}(H) = \mathcal{H}^2$. Also, it is well known [43, Thm. 12.1] that the wave operators $W_\pm$ exist and are asymptotically complete. In stationary scattering theory one defines the wave operators in terms of suitable limits of the resolvents of H_0 and H on the real axis. We shall mainly use this second approach, noting that for this model both definitions for the wave operators do coincide (see [57, Sec. 5.3]).

Let us thus recall from [57, Eq. 2.7.5] that for suitable $f, g \in \mathcal{H}$ the stationary expressions for the wave operators are given by[6]

$$\big\langle W_\pm f, g\big\rangle_{\mathcal{H}} = \int_{\mathbb{R}} \mathrm{d}\lambda \lim_{\varepsilon \searrow 0} \frac{\varepsilon}{\pi}\big\langle R_0(\lambda \pm i\varepsilon) f, R(\lambda \pm i\varepsilon) g\big\rangle_{\mathcal{H}},$$

where $R_0(z) := (H_0 - z)^{-1}$ and $R(z) := (H - z)^{-1}$, $z \in \mathbb{C} \setminus \mathbb{R}$, are the resolvents of the operators H_0 and H. We also recall from [57, Sec. 1.4] that the limit $\lim_{\varepsilon \searrow 0}\big\langle \delta_\varepsilon(H_0 - \lambda) f, g\big\rangle_{\mathcal{H}}$ with $\delta_\varepsilon(H_0 - \lambda) := \frac{\varepsilon}{\pi} R_0(\lambda \mp i\varepsilon)\, R_0(\lambda \pm i\varepsilon)$ exists for a.e. $\lambda \in \mathbb{R}$ and that

$$\big\langle f, g\big\rangle_{\mathcal{H}} = \int_{\mathbb{R}} \mathrm{d}\lambda \lim_{\varepsilon \searrow 0}\big\langle \delta_\varepsilon(H_0 - \lambda) f, g\big\rangle_{\mathcal{H}}.$$

[6] In this section, the various scalar products are indexed by the corresponding Hilbert spaces.

Thus, taking into account the second resolvent equation, one infers that

$$\big\langle (W_\pm - 1)f, g\big\rangle_{\mathcal H} = -\int_{\mathbb R} \mathrm d\lambda \lim_{\varepsilon\searrow 0} \big\langle \delta_\varepsilon(H_0-\lambda)f, \big(1+VR_0(\lambda\pm i\varepsilon)\big)^{-1} VR_0(\lambda\pm i\varepsilon)g\big\rangle_{\mathcal H}.$$

We now derive expressions for the wave operators in the spectral representation of H_0; that is, for the operators $\mathscr F_0(W_\pm - 1)\mathscr F_0^*$. So, let φ,ψ be suitable elements of $\mathscr H$ (precise conditions will be specified in Theorem 6.7 below), then one obtains that

$$\begin{aligned}
&\big\langle \mathscr F_0(W_\pm - 1)\mathscr F_0^*\varphi,\psi\big\rangle_{\mathscr H}\\
&\quad = -\int_{\mathbb R}\mathrm d\lambda \lim_{\varepsilon\searrow 0}\big\langle V\big(1+R_0(\lambda\mp i\varepsilon)V\big)^{-1}\mathscr F_0^*\,\delta_\varepsilon(L-\lambda)\varphi, \mathscr F_0^*\,(L-\lambda\mp i\varepsilon)^{-1}\psi\big\rangle_{\mathcal H}\\
&\quad = -\int_{\mathbb R}\mathrm d\lambda \lim_{\varepsilon\searrow 0}\int_0^\infty \mathrm d\mu\,\big\langle\big\{\mathscr F_0 V\big(1+R_0(\lambda\mp i\varepsilon)V\big)^{-1}\\
&\qquad\qquad\qquad\qquad \times \mathscr F_0^*\,\delta_\varepsilon(L-\lambda)\varphi\big\}(\mu), (\mu-\lambda\mp i\varepsilon)^{-1}\psi(\mu)\big\rangle_{\mathfrak h}.
\end{aligned}$$

Using the shorthand notation $T(z) := V\big(1+R_0(z)V\big)^{-1}$, $z\in\mathbb C\setminus\mathbb R$, one thus gets the equality

$$\begin{aligned}
&\big\langle \mathscr F_0(W_\pm - 1)\mathscr F_0^*\varphi,\psi\big\rangle_{\mathscr H}\\
&= -\int_{\mathbb R}\mathrm d\lambda \lim_{\varepsilon\searrow 0}\int_0^\infty \mathrm d\mu\,\big\langle\big\{\mathscr F_0\,T(\lambda\mp i\varepsilon)\,\mathscr F_0^*\,\delta_\varepsilon(L-\lambda)\varphi\big\}(\mu), (\mu-\lambda\mp i\varepsilon)^{-1}\psi(\mu)\big\rangle_{\mathfrak h}.
\end{aligned}\tag{6.2}$$

This formula will be our starting point for computing new expressions for the wave operators. The next step is to exchange the integral over μ and the limit $\varepsilon\searrow 0$. To do it properly, we need a series of preparatory lemmas. First of all, we recall that for $\lambda>0$ the trace operator $\gamma(\lambda)$ extends to an element of $\mathcal B(\mathcal H^s_t,\mathfrak h)$ for each $s>1/2$ and $t\in\mathbb R$, where $\mathcal H^s_t=\mathcal H^s_t(\mathbb R^3)$ denotes the weighted Sobolev space over $\mathbb R^3$ with index $s\in\mathbb R$ and with the index $t\in\mathbb R$ associated with the weight[7]. In addition, the map $\mathbb R_+\ni\lambda\mapsto\gamma(\lambda)\in\mathcal B(\mathcal H^s_t,\mathfrak h)$ is continuous, see for example [24, Sec. 3]. As a consequence, the operator $\mathscr F_0(\lambda):\mathcal S(\mathbb R^3)\to\mathfrak h$ given by $\mathscr F_0(\lambda)f := (\mathscr F_0 f)(\lambda)$ extends to an element of $\mathcal B(\mathcal H^s_t,\mathfrak h)$ for each $s\in\mathbb R$ and $t>1/2$, and the map $\mathbb R_+\ni\lambda\mapsto\mathscr F_0(\lambda)\in\mathcal B(\mathcal H^s_t,\mathfrak h)$ is continuous.

We recall now three technical lemmas which have been proved in [47] and which strengthen some standard results.

Lemma 6.2. *Let $s\geq 0$ and $t>3/2$. Then, the functions*

$$(0,\infty)\ni\lambda\mapsto\lambda^{\pm 1/4}\mathscr F_0(\lambda)\in\mathcal B(\mathcal H^s_t,\mathfrak h)$$

are continuous and bounded.

One immediately infers from Lemma 6.2 that the function

$$\mathbb R_+\ni\lambda\mapsto\|\mathscr F_0(\lambda)\|_{\mathcal B(\mathcal H^s_t,\mathfrak h)}\in\mathbb R$$

[7] We also use the convention $\mathcal H^s=\mathcal H^s_0$ and $\mathcal H_t=\mathcal H^0_t$.

is continuous and bounded for any $s \geq 0$ and $t > 3/2$. Also, one can strengthen the statement of Lemma 6.2 in the case of the minus sign:

Lemma 6.3. *Let $s > -1$ and $t > 3/2$. Then, $\mathscr{F}_0(\lambda) \in \mathcal{K}(\mathcal{H}_t^s, \mathfrak{h})$ for each $\lambda \in \mathbb{R}_+$, and the function $\mathbb{R}_+ \ni \lambda \mapsto \lambda^{-1/4}\mathscr{F}_0(\lambda) \in \mathcal{K}(\mathcal{H}_t^s, \mathfrak{h})$ is continuous, admits a limit as $\lambda \searrow 0$ and vanishes as $\lambda \to \infty$.*

From now on, we use the notation $C_c(\mathbb{R}_+; \mathcal{G})$ for the set of compactly supported and continuous functions from $\mathbb{R}_+$ to some Hilbert space $\mathcal{G}$.

With this notation and what precedes, we note that the multiplication operator $M : C_c(\mathbb{R}_+; \mathcal{H}_t^s) \to \mathscr{H}$ given by

$$(M\xi)(\lambda) := \lambda^{-1/4}\mathscr{F}_0(\lambda)\xi(\lambda), \quad \xi \in C_c(\mathbb{R}_+; \mathcal{H}_t^s),\ \lambda \in \mathbb{R}_+, \tag{6.3}$$

extends for $s \geq 0$ and $t > 3/2$ to an element of $\mathcal{B}\big(\mathsf{L}^2(\mathbb{R}_+; \mathcal{H}_t^s), \mathscr{H}\big)$.

The next step is to deal with the limit $\varepsilon \searrow 0$ of the operator $\delta_\varepsilon(L - \lambda)$ in Equation (6.2). For that purpose, we shall use the continuous extension of the scalar product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ to a duality $\langle \cdot, \cdot \rangle_{\mathcal{H}_t^s, \mathcal{H}_{-t}^{-s}}$ between $\mathcal{H}_t^s$ and $\mathcal{H}_{-t}^{-s}$.

Lemma 6.4. *Take $s \geq 0$, $t > 3/2$, $\lambda \in \mathbb{R}_+$ and $\varphi \in C_c(\mathbb{R}_+; \mathfrak{h})$. Then, we have*

$$\lim_{\varepsilon \searrow 0} \big\| \mathscr{F}_0^* \, \delta_\varepsilon(L - \lambda)\varphi - \mathscr{F}_0(\lambda)^* \varphi(\lambda) \big\|_{\mathcal{H}_{-t}^{-s}} = 0.$$

The next necessary result concerns the limits $T(\lambda \pm i0) := \lim_{\varepsilon \searrow 0} T(\lambda \pm i\varepsilon)$, $\lambda \in \mathbb{R}_+$. Fortunately, it is already known (see for example [26, Lemma 9.1]) that if $\rho > 1$ in (6.1) then the limit $\big(1 + R_0(\lambda + i0)V\big)^{-1} := \lim_{\varepsilon \searrow 0} \big(1 + R_0(\lambda + i\varepsilon)V\big)^{-1}$ exists in $\mathcal{B}(\mathcal{H}_{-t}, \mathcal{H}_{-t})$ for any $t \in (1/2, \rho - 1/2)$, and that the map $\mathbb{R}_+ \ni \lambda \mapsto \big(1 + R_0(\lambda + i0)V\big)^{-1} \in \mathcal{B}(\mathcal{H}_{-t}, \mathcal{H}_{-t})$ is continuous. Corresponding results for $T(\lambda + i\varepsilon)$ follow immediately. Note that only the limits from the upper half-plane have been computed in [26], even though similar results for $T(\lambda - i0)$ could have been derived. Due to this lack of information in the literature and for the simplicity of the exposition, we consider from now on only the wave operator W_-.

Proposition 6.5. *Take $\rho > 5$ in (6.1) and let $t \in (5/2, \rho - 5/2)$. Then, the function*

$$\mathbb{R}_+ \ni \lambda \mapsto \lambda^{1/4} T(\lambda + i0)\mathscr{F}_0(\lambda)^* \in \mathcal{B}(\mathfrak{h}, \mathcal{H}_{\rho - t})$$

is continuous and bounded, and the multiplication operator $B : C_c\big(\mathbb{R}_+; \mathfrak{h}\big) \to \mathsf{L}^2(\mathbb{R}_+; \mathcal{H}_{\rho - t})$ given by

$$(B\varphi)(\lambda) := \lambda^{1/4} T(\lambda + i0)\mathscr{F}_0(\lambda)^* \varphi(\lambda) \in \mathcal{H}_{\rho - t}, \quad \varphi \in C_c\big(\mathbb{R}_+; \mathfrak{h}\big),\ \lambda \in \mathbb{R}_+, \tag{6.4}$$

extends to an element of $\mathcal{B}\big(\mathscr{H}, \mathsf{L}^2(\mathbb{R}_+; \mathcal{H}_{\rho - t})\big)$.

Remark 6.6. If one assumes that H has no 0-energy eigenvalue and/or no 0-energy resonance, then one can prove Proposition 6.5 under a weaker assumption on the decay of V at infinity. However, even if the absence of 0-energy eigenvalue and 0-energy resonance is generic, we do not want to make such an implicit assumption in the sequel. The condition on V is thus imposed adequately.

We are ready for stating the main result of this section. Let us simply recall that the dilation group in $\mathsf{L}^2(\mathbb{R}_+)$ has been introduced in (2.1) and that A denotes its generator. We also recall that the Hilbert spaces $\mathsf{L}^2(\mathbb{R}_+;\mathcal{H}^s_t)$ and $\mathscr{H}$ can be naturally identified with the Hilbert spaces $\mathsf{L}^2(\mathbb{R}_+)\otimes\mathcal{H}^s_t$ and $\mathsf{L}^2(\mathbb{R}_+)\otimes\mathfrak{h}$.

Theorem 6.7. *Take $\rho>7$ in* (6.1) *and let $t\in(7/2,\rho-7/2)$. Then, one has in $\mathcal{B}(\mathscr{H})$ the equality*

$$\mathscr{F}_0(W_- -1)\,\mathscr{F}_0^* = -2\pi i\,M\left\{\tfrac{1}{2}\big(1-\tanh(2\pi A)-i\cosh(2\pi A)^{-1}\big)\otimes 1_{\mathcal{H}_{\rho-t}}\right\}B,$$

with M and B defined in (6.3) *and* (6.4).

The proof of this statement is rather technical and we shall not reproduce it here. Let us however mention the key idea. Consider $\varphi\in C_{\mathrm{c}}(\mathbb{R}_+;\mathfrak{h})$ and $\psi\in C_{\mathrm{c}}^\infty(\mathbb{R}_+)\odot C(\mathbb{S}^2)$ (the algebraic tensor product), and set $s:=\rho-t>7/2$. Then, we have for each $\varepsilon>0$ and $\lambda\in\mathbb{R}_+$ the inclusions

$$g_\varepsilon(\lambda):=\lambda^{1/4}\,T(\lambda+i\varepsilon)\,\mathscr{F}_0^*\,\delta_\varepsilon(L-\lambda)\varphi\in\mathcal{H}_s$$

and

$$f(\lambda):=\lambda^{-1/4}\mathscr{F}_0(\lambda)^*\psi(\lambda)\in\mathcal{H}_{-s}\,.$$

It follows that the expression (6.2) is equal to

$$\begin{aligned}&-\int_{\mathbb{R}}\mathrm{d}\lambda\,\lim_{\varepsilon\searrow 0}\int_0^\infty\mathrm{d}\mu\,\big\langle T(\lambda+i\varepsilon)\,\mathscr{F}_0^*\,\delta_\varepsilon(L-\lambda)\varphi,(\mu-\lambda+i\varepsilon)^{-1}\,\mathscr{F}_0(\mu)^*\,\psi(\mu)\big\rangle_{\mathcal{H}_s,\mathcal{H}_{-s}}\\ &\quad=-\int_{\mathbb{R}_+}\mathrm{d}\lambda\,\lim_{\varepsilon\searrow 0}\int_0^\infty\mathrm{d}\mu\,\left\langle g_\varepsilon(\lambda),\frac{\lambda^{-1/4}\mu^{1/4}}{\mu-\lambda+i\varepsilon}\,f(\mu)\right\rangle_{\mathcal{H}_s,\mathcal{H}_{-s}}.\end{aligned}$$

Then, once the exchange between the limit $\varepsilon\searrow 0$ and the integral with variable μ has been fully justified, one obtains that

$$\big\langle\mathscr{F}_0(W_\pm-1)\mathscr{F}_0^*\varphi,\psi\big\rangle_{\mathscr{H}}=-\int_{\mathbb{R}_+}\mathrm{d}\lambda\int_0^\infty\mathrm{d}\mu\,\left\langle g_0(\lambda),\frac{\lambda^{-1/4}\mu^{1/4}}{\mu-\lambda+i0}\,f(\mu)\right\rangle_{\mathcal{H}_s,\mathcal{H}_{-s}}.$$

It remains to observe that $g_0(\lambda)=[B\varphi](\lambda)$ and that $f=M^*\psi$, and to derive a nice function of A from the kernel $\frac{\lambda^{-1/4}\mu^{1/4}}{\mu-\lambda+i0}$. We refer to the proof of [47, Thm. 2.6] for the details.

The next result is a technical lemma which asserts that a certain commutator is compact. Its proof is mainly based on a result of Cordes which states that if $f_1,f_2\in C([-\infty,\infty])$, then the following inclusion holds: $[f_1(X),f_2(D)]\in\mathcal{K}\big(\mathsf{L}^2(\mathbb{R})\big)$. By conjugating this inclusion with the Mellin transform as introduced in Section 4.4, one infers that $\big[f_1(A),f_3(L)\big]\in\mathcal{K}\big(\mathsf{L}^2(\mathbb{R}_+)\big)$ with $f_3:=f_2\circ(-\ln)\in C([0,\infty])$. Note finally that the following statement does not involve the potential V, but only some operators which are related to $-\Delta$ and to its spectral representation.

Lemma 6.8. *Take $s > -1$ and $t > 3/2$. Then, the difference*

$$\big\{\big(\tanh(2\pi A)+i\cosh(2\pi A)^{-1}\big)\otimes 1_{\mathfrak{h}}\big\}M - M\big\{\big(\tanh(2\pi A)+i\cosh(2\pi A)^{-1}\big)\otimes 1_{\mathcal{H}^s_t}\big\}$$

belongs to $\mathcal{K}\big(\mathsf{L}^2(\mathbb{R}_+;\mathcal{H}^s_t),\mathscr{H}\big)$.

Before providing the proof of Theorem 6.1, let us simply mention that the following equality holds:

$$\tfrac{1}{2}\big(1+\tanh(\pi A)-i\cosh(\pi A)^{-1}\big) = \mathscr{F}_0^*\big\{\tfrac{1}{2}\big(1-\tanh(2\pi A)-i\cosh(2\pi A)^{-1}\big)\otimes 1_{\mathfrak{h}}\big\}\mathscr{F}_0.$$

with the generator of dilations on $\mathbb{R}^3$ in the l.h.s. and the generator of dilations on $\mathbb{R}_+$ in the r.h.s.

Proof of Theorem 6.1. Set $s = 0$ and $t \in (7/2, \rho - 7/2)$. Then, we deduce from Theorem 6.7, Lemma 6.8 and the above paragraph that

$$\begin{aligned} W_- - 1 &= -2\pi i\mathscr{F}_0^* M\big\{\tfrac{1}{2}\big(1-\tanh(2\pi A)-i\cosh(2\pi A)^{-1}\big)\otimes 1_{\mathcal{H}_{\rho-t}}\big\}B\mathscr{F}_0 \\ &= -2\pi i\mathscr{F}_0^*\big\{\tfrac{1}{2}\big(1-\tanh(2\pi A)-i\cosh(2\pi A)^{-1}\big)\otimes 1_{\mathfrak{h}}\big\}MB\mathscr{F}_0 + K \\ &= \tfrac{1}{2}\big(1+\tanh(\pi A)-i\cosh(\pi A)^{-1}\big)\mathscr{F}_0^*(-2\pi iMB)\mathscr{F}_0 + K, \end{aligned} \quad (6.5)$$

with $K \in \mathcal{K}(\mathcal{H})$. Comparing $-2\pi iMB$ with the usual expression for the scattering matrix $S(\lambda)$ (see for example [26, Eq. (5.1)]), one observes that $-2\pi iMB = \int_{\mathbb{R}_+}^{\oplus}\mathrm{d}\lambda\,\big(S(\lambda)-1\big)$. Since $\mathscr{F}_0$ defines the spectral representation of H_0, one obtains that

$$W_- - 1 = \tfrac{1}{2}\big(1+\tanh(\pi A)-i\cosh(\pi A)^{-1}\big)[S-1]+K. \quad (6.6)$$

The formula for $W_+ - 1$ follows then from (6.6) and the relation $W_+ = W_- S^*$. □

6.2. The index theorem

In order to figure out the algebraic framework necessary for this model, let us first look again at the wave operator in the spectral representation of H_0. More precisely, one deduces from (6.5) that the following equality holds in $\mathscr{H} \equiv \mathsf{L}^2(\mathbb{R}_+)\otimes\mathfrak{h}$:

$$\mathscr{F}_0 W_-\mathscr{F}_0^* = 1 + \big\{\tfrac{1}{2}\big(1-\tanh(2\pi A)-i\cosh(2\pi A)^{-1}\big)\otimes 1_{\mathfrak{h}}\big\}[S(L)-1]+K$$

with $K \in \mathcal{K}(\mathscr{H})$. Secondly, let us recall some information on the scattering matrix which are available in the literature. Under the assumption on V imposed in Theorem 6.1, the map

$$\mathbb{R}_+ \ni \lambda \mapsto S(\lambda) - 1 \in \mathcal{K}_2(\mathfrak{h})$$

is continuous, where $\mathcal{K}_2(\mathfrak{h})$ denotes the set of Hilbert–Schmidt operators on $\mathfrak{h}$, endowed with the Hilbert–Schmidt norm. A fortiori, this map is continuous in the norm topology of $\mathcal{K}(\mathfrak{h})$, and in fact this map belongs to $C\big([0,+\infty];\mathcal{K}(\mathfrak{h})\big)$. Indeed, it is well known that $S(\lambda)$ converges to 1 as $\lambda \to \infty$, see for example [4, Prop. 12.5]. For the low energy behavior, see [26] where the norm convergence of $S(\lambda)$ for $\lambda \to 0$ is proved (under conditions on V which are satisfied in our Theorem 6.1). The picture is the following: If H does not possess a 0-energy resonance, then $S(0)$ is equal to 1, but if such a resonance exists, then $S(0)$ is equal to $1-2P_0$, where P_0 denotes the orthogonal projection on the one-dimensional subspace of spherically symmetric functions in $\mathfrak{h} \equiv \mathsf{L}^2(\mathbb{S}^2)$.

By taking these information into account, it is natural to define the unital C^*-subalgebra $\mathcal{E}'$ of $\mathcal{B}\big(\mathsf{L}^2(\mathbb{R}_+)\otimes\mathfrak{h}\big)$ by $\mathcal{E}' := \big\{\mathcal{E}_{(L,A)}\otimes\mathcal{K}(\mathfrak{h})\big\}^+$ and to consider the short exact sequence

$$0 \to \mathcal{K}\big(\mathsf{L}^2(\mathbb{R}_+)\big)\otimes\mathcal{K}(\mathfrak{h}) \hookrightarrow \mathcal{E}' \xrightarrow{q} \big\{C(\square)\otimes\mathcal{K}(\mathfrak{h})\big\}^+ \to 0.$$

However, we prefer to look at a unitarily equivalent representation of this algebra in the original Hilbert space $\mathcal{H}$, and set $\mathcal{E} := \mathscr{F}_0^*\big\{\mathcal{E}_{(L,A)}\otimes\mathcal{K}(\mathfrak{h})\big\}^+\mathscr{F}_0 \subset \mathcal{B}(\mathcal{H})$. The corresponding short exact sequence reads

$$0 \to \mathcal{K}(\mathcal{H}) \hookrightarrow \mathcal{E} \xrightarrow{q} \big\{C(\square)\otimes\mathcal{K}(\mathfrak{h})\big\}^+ \to 0,$$

and this framework is the suitable one for the next statement:

Corollary 6.9. *Let $V \in \mathsf{L}^\infty(\mathbb{R}^3)$ be real and satisfy $|V(x)| \leq \text{Const.}\,(1+|x|)^{-\rho}$ with $\rho > 7$ for almost every $x \in \mathbb{R}^3$. Then W_- belongs to $\mathcal{E}$ and its image $\Gamma_\square := q(W_-)$ in $\big\{C(\square)\otimes\mathcal{K}(\mathfrak{h})\big\}^+$ is given by*

$$\Gamma_\square = \Big(1 + \tfrac{1}{2}\big(1+\tanh(\pi\cdot) - i\cosh(\pi\cdot)^{-1}\big)[S(0)-1], S(\cdot), 1, 1\Big).$$

In addition, the equality

$$\operatorname{ind}[\Gamma_\square]_1 = -[E_{\mathrm{p}}(H)]_0 \tag{6.7}$$

holds, with $[\Gamma_\square]_1 \in K_1\big(\big\{C(\square)\otimes\mathcal{K}(\mathfrak{h})\big\}^+\big)$ and $[E_{\mathrm{p}}(H)]_0 \in K_0\big(\mathcal{K}(\mathcal{H})\big)$.

Let us mention again that if H has no 0-energy resonance, then $S(0)-1$ is equal to 0, and thus the first term Γ_1 in the quadruple $\Gamma_\square$ is equal to 1. However, if such a resonance exists, then Γ_1 is not equal to 1 but to

$$1 - \big(1+\tanh(\pi\cdot) - i\cosh(\pi\cdot)^{-1}\big)P_0 = P_0^\perp + \big(-\tanh(\pi\cdot) + i\cosh(\pi\cdot)^{-1}\big)P_0.$$

This term will allow us to explain the correction which often appears in the literature for 3-dimensional Schrödinger operators in the presence of a resonance at 0. However, for that purpose we first need a concrete computable version of our topological Levinson theorem, or in other words a way to deduce an equality between numbers from the equality (6.7).

The good point in the previous construction is that the K_0-group of $\mathcal{K}(\mathcal{H})$ and the K_1-group of $\big\{C(\square)\otimes\mathcal{K}(\mathfrak{h})\big\}^+$ are both isomorphic to $\mathbb{Z}$. On the other hand, since $S(\lambda)-1$ takes values in $\mathcal{K}(\mathfrak{h})$ and not in $\mathcal{M}_n(\mathbb{C})$ for some fixed n, it is not possible to simply apply the map Wind without a regularization process. In the next section, we shall explain how such a regularization can be constructed, but let us already present the final result for this model.

In the following statement, we shall use the fact that for the class of perturbations we are considering the map $\mathbb{R}_+ \ni \lambda \mapsto S(\lambda)-1 \in \mathcal{K}(\mathfrak{h})$ is continuous in the Hilbert–Schmidt norm. Furthermore, it is known that this map is even continuously differentiable in the norm topology. In particular, the on-shell time delay operator $i\,S(\lambda)^*\,S'(\lambda)$ is well defined for each $\lambda \in \mathbb{R}_+$, see [24, 25] for details. If we set $\mathcal{K}_1(\mathfrak{h})$ for the trace class operators in $\mathcal{K}(\mathfrak{h})$, and denote the corresponding trace by tr, then the following statement holds:

Theorem 6.10. *Let $V \in \mathsf{L}^\infty(\mathbb{R}^3)$ be real and satisfy $|V(x)| \leq \text{Const.}\,(1+|x|)^{-\rho}$ with $\rho > 7$ for almost every $x \in \mathbb{R}^3$. Then for any $p \geq 2$ one has*

$$\frac{1}{2\pi}\bigg\{\int_{-\infty}^{\infty} \operatorname{tr}\big[i\big(1-\Gamma_1(\xi)\big)^p\Gamma_1(\xi)^*\,\Gamma_1'(\xi)\big]\,\mathrm{d}\xi + \int_0^\infty \operatorname{tr}\big[i\big(1-S(\lambda)\big)^p S(\lambda)^*\,S'(\lambda)\big]\,\mathrm{d}\lambda\bigg\} = \sharp\sigma_{\mathrm{p}}(H).$$

In addition, if the map $\lambda \mapsto S(\lambda)-1$ is continuously differentiable in the Hilbert–Schmidt norm, then the above equality holds also for any $p \geq 1$.

The proof of this statement is a corollary of the construction presented in the next section. For completeness, let us mention that in the absence of a resonance at 0 for H, in which case $\Gamma_1 = 1$, only the second term containing $S(\cdot)$ contributes to the l.h.s. On the other hand, in the presence of a resonance at 0 the real part of the integral of the term Γ_1 yields

$$\operatorname{Re}\bigg\{\frac{1}{2\pi}\int_{-\infty}^{\infty} \operatorname{tr}\big[i\big(1-\Gamma_1(\xi)\big)^p\Gamma_1(\xi)^*\,\Gamma_1'(\xi)\big]\,\mathrm{d}\xi\bigg\} = -\tfrac{1}{2}$$

which accounts for the correction usually found in Levinson's theorem. Note that only the real part of this expression is of interest since its imaginary part will cancel with the corresponding imaginary part of term involving $S(\cdot)$.

6.3. A regularization process

In this section and in the corresponding part of the Appendix, we recall and adapt some of the results and proofs from [32] on a regularization process. More precisely, for an arbitrary Hilbert space $\mathfrak{h}$, we consider a unitary element $\Gamma \in C\big(\mathbb{S};\mathcal{K}(\mathfrak{h})\big)^+$ of the form $\Gamma(t) - 1 \in \mathcal{K}(\mathfrak{h})$ for any $t \in \mathbb{S}$. Clearly, there is a certain issue about the possibility of computing a kind of winding number on this element, as the determinant of $\Gamma(t)$ is not always defined. Nevertheless, at the level of K-theory, it is *a priori* possible to define Wind on $[\Gamma]_1$ simply by evaluating it on a representative on which the pointwise determinant is well defined and depends continuously on t. For our purpose this approach is not sufficient, however, as it is not clear how to construct for a given Γ such a representative. We will therefore have to make recourse to a regularization of the determinant.

Let us now explain this regularization in the case that $\Gamma(t) - 1$ lies in the pth Schatten ideal $\mathcal{K}_p(\mathfrak{h})$ for some integer p, that is, $|\Gamma(t)-1|^p$ belongs to $\mathcal{K}_1(\mathfrak{h})$. We also denote by $\{e^{i\theta_j(t)}\}_j$ the set of eigenvalues of $\Gamma(t)$. Then the regularized Fredholm determinant $\det_p$, defined by [20, Eq. (XI.4.5)]

$$\det{}_p\big(\Gamma(t)\big) = \prod_j e^{i\theta_j(t)} \exp\left(\sum_{k=1}^{p-1} \frac{(-1)^k}{k}\big(e^{i\theta_j(t)}-1\big)^k\right)$$

is finite and non-zero. Thus, if in addition we suppose that $t \mapsto \Gamma(t) - 1$ is continuous in the pth Schatten norm, then the map $t \to \det_p\big(\Gamma(t)\big)$ is continuous and hence the winding number of the map $\mathbb{S} \ni t \mapsto \det_p\big(\Gamma(t)\big) \in \mathbb{C}^*$ can be defined. However, in order to get an analytic formula for this winding number, stronger conditions are necessary, as explicitly required in the following statements:

Lemma 6.11. *Let $I \subset \mathbb{S}$ be an open arc of the unit circle, and assume that the map $I \ni t \mapsto \Gamma(t) - 1 \in \mathcal{K}_p(\mathfrak{h})$ is continuous in norm of $\mathcal{K}_p(\mathfrak{h})$ and is continuously differentiable in norm of $\mathcal{K}(\mathfrak{h})$. Then the map $I \ni t \mapsto \det_{p+1}\big(\Gamma(t)\big) \in \mathbb{C}$ is continuously differentiable and the following equality holds for any $t \in I$:*

$$\Big(\ln \det_{p+1}\big(\Gamma(\cdot)\big)\Big)'(t) = \operatorname{tr}\big[\big(1 - \Gamma(t)\big)^p \Gamma(t)^* \Gamma'(t)\big]. \qquad (6.8)$$

Furthermore, if the map $I \ni t \mapsto \Gamma(t) - 1 \in \mathcal{K}_p(\mathfrak{h})$ is continuously differentiable in norm of $\mathcal{K}_p(\mathfrak{h})$, then the statement already holds for p instead of $p + 1$.

The proof of this statement is provided in Section 9.2. Based on (6.8), it is natural to define

$$\operatorname{Wind}(\Gamma) := \frac{1}{2\pi} \int_{\mathbb{S}} \operatorname{tr}\big[i\big(1 - \Gamma(t)\big)^p \Gamma(t)^* \Gamma'(t)\big] \mathrm{d}t$$

whenever the integrand is well defined and integrable. However, such a definition is meaningful only if the resulting number does not depend on p, for sufficiently large p. This is indeed the case, as shown in the next statement:

Lemma 6.12. *Assume that the map $\mathbb{S} \ni t \mapsto \Gamma(t) - 1 \in \mathcal{K}_p(\mathfrak{h})$ is continuous in norm of $\mathcal{K}_p(\mathfrak{h})$, and that this map is continuously differentiable in norm of $\mathcal{K}(\mathfrak{h})$, except on a finite subset of $\mathbb{S}$ (which can be void). If the map $t \mapsto \operatorname{tr}\big[i\big(1 - \Gamma(t)\big)^p \Gamma(t)^* \Gamma'(t)$ is integrable for some integer p, then for any integer $q > p$ one has:*

$$\frac{1}{2\pi} \int_{\mathbb{S}} \operatorname{tr}\big[i\big(1 - \Gamma(t)\big)^q \Gamma(t)^* \Gamma'(t)\big] \mathrm{d}t = \frac{1}{2\pi} \int_{\mathbb{S}} \operatorname{tr}\big[i\big(1 - \Gamma(t)\big)^p \Gamma(t)^* \Gamma'(t)\big] \mathrm{d}t\ .$$

The proof of this statement is again provided in Section 9.2. Clearly, Theorem 6.10 is an application of the previous lemma with $p = 2$.

Before ending this section, let us add one illustrative example. In it, the problem does not come from the computation of a determinant, but from an integrability condition. More precisely, for any $a, b > 0$ we consider $\varphi_{a,b} : [0, 1] \to \mathbb{R}$ defined by

$$\varphi_{a,b}(x) = x^a \sin\big(\pi x^{-b}/2\big), \qquad x \in [0, 1].$$

Let us also set $\Gamma_{a,b} : [0, 2\pi] \to \mathbb{T}$ by

$$\Gamma_{a,b}(x) := \mathrm{e}^{-2\pi i \varphi_{a,b}(x/2\pi)}\ .$$

Clearly, $\Gamma_{a,b}$ is continuous on $[0, 2\pi]$ with $\Gamma_{a,b}(0) = \Gamma_{a,b}(2\pi)$, and thus can be considered as an element of $C(\mathbb{S})$. In addition, $\Gamma_{a,b}$ is unitary, and thus there exists an element $[\Gamma_{a,b}]_1$ in $K_1\big(C(\mathbb{S})\big)$. One easily observes that the equality $[\mathrm{e}^{-2\pi i\,\mathrm{id}}]_1 = [\Gamma_{a,b}]_1$ holds, meaning that the equivalence class $[\Gamma_{a,b}]$ contains the simpler function $x \mapsto \mathrm{e}^{-2\pi i x}$. However, the same equivalence class also contains some functions which are continuous but not differentiable at a finite number of points, or even wilder continuous functions.

Now, the computation of the winding number of any of these functions can be performed by a topological argument, and one obtains

$$\mathrm{Wind}_t(\Gamma_{a,b}) := \varphi_{a,b}(1) - \varphi_{a,b}(0) = 1.$$

Here, we have added an index t for emphasizing that this number is computed *topologically.* On the other hand, if one is interested in an explicit analytical formula for this winding number, one immediately faces some troubles. Namely, let us first observe that for $x \neq 0$

$$\varphi'_{a,b}(x) = ax^{a-1}\sin\left(\pi x^{-b}/2\right) - \frac{b\pi}{2}x^{a-b-1}\cos\left(\pi x^{-b}/2\right).$$

Clearly, the first term is integrable for any $a, b > 0$ while the second one is integrable only if $a > b$. Thus, in such a case it is natural to set

$$\begin{aligned}\mathrm{Wind}_a(\Gamma_{a,b}) &:= \frac{1}{2\pi}\int_0^{2\pi} i\Gamma_{a,b}(x)^*\Gamma'_{a,b}(x)\mathrm{d}x \\ &= \frac{1}{2\pi}\int_0^{2\pi}\varphi'_{a,b}(x/2\pi)\mathrm{d}x = \int_0^1\varphi'_{a,b}(x)\mathrm{d}x\end{aligned}$$

and this formula is well defined, even if one looks at each term of $\varphi'_{a,b}$ separately. Note that in this formula, the index a stands for *analytic*. Finally, in the case $b \geq a > 0$ the previous formula is not well defined if one looks at both terms separately, but one can always find $p \in \mathbb{N}$ such that $(p+1)a > b$. Then one can set

$$\begin{aligned}\mathrm{Wind}_r(\Gamma_{a,b}) &:= \frac{1}{2\pi}\int_0^{2\pi}\left(1 - \Gamma_{a,b}(x)\right)^p i\Gamma_{a,b}(x)^*\Gamma'_{a,b}(x)\mathrm{d}x \\ &= \frac{1}{2\pi}\int_0^{2\pi}\left(1 - \Gamma_{a,b}(x)\right)^p\varphi'_{a,b}(x/2\pi)\mathrm{d}x \\ &= \int_0^1\left(1 - \Gamma_{a,b}(2\pi x)\right)^p\varphi'_{a,b}(x)\mathrm{d}x,\end{aligned}$$

and this formula is well defined, even if one looks at each term of $\varphi'_{a,b}$ separately. Note that here the index r stands for *regularized.* Clearly, the value which can be obtained from these formulas is always equal to 1.

7. Schrödinger operators on $\mathbb{R}^2$

In this section, we simply provide an explicit formula for the wave operators in the context of Schrödinger operators on $\mathbb{R}^2$. The statement is very similar to the one presented in Section 6.1, and its proof is based on the same scheme. We refer to [48] for a more detailed presentation of the result and for its proof. Let us however mention that some technicalities have not been considered in $\mathbb{R}^2$, and therefore our main result applies only in the absence of 0-energy bound state or 0-energy resonance.

Let us be more precise about the framework. In the Hilbert space $\mathsf{L}^2(\mathbb{R}^2)$ we consider the Schrödinger operator $H_0 := -\Delta$ and the perturbed operator $H := -\Delta + V$, with a potential $V \in \mathsf{L}^\infty(\mathbb{R}^2;\mathbb{R})$ decaying fast enough at infinity. In such a situation, it is well known that the wave operators $W_\pm$ for the pair (H, H_0) exist and are asymptotically complete. As a consequence, the scattering operator $S := W_+^* W_-$ is a unitary operator.

Theorem 7.1. *Suppose that $V \in \mathsf{L}^\infty(\mathbb{R}^2)$ is real and satisfies $|V(x)| \leq \mathrm{Const.}\,(1+|x|)^{-\rho}$ with $\rho > 11$ for almost every $x \in \mathbb{R}^2$, and assume that H has neither eigenvalues nor resonances at 0-energy. Then, one has in $\mathcal{B}\big(\mathsf{L}^2(\mathbb{R}^2)\big)$ the equalities*

$$W_- = 1 + \tfrac{1}{2}\big(1 + \tanh(\pi A/2)\big)[S - 1] + K$$

and

$$W_+ = 1 + \tfrac{1}{2}\big(1 - \tanh(\pi A/2)\big)[S^* - 1] + K',$$

with A the generator of dilations in $\mathsf{L}^2(\mathbb{R}^2)$ and $K, K' \in \mathcal{K}\big(\mathsf{L}^2(\mathbb{R}^2)\big)$.

We stress that the absence of eigenvalues or resonances at 0-energy is generic. Their presence leads to slightly more complicated expressions and this has not been considered in [48]. On the other hand, we note that no spherical symmetry is imposed on V. Note also that in the mentioned reference, an additional formula for $W_\pm$ which does not involve any compact remainder (as in Theorem 6.7) has been exhibited. For this model, we do not deduce any topological Levinson theorem, since this has already been performed for the 3-dimensional case, and since the exceptional case has not yet been fully investigated. Let us however mention that similar results already exist in the literature, but that the approaches are completely different. We refer to [7, 17, 18, 27, 52, 58] for more information on this model and for related results.

8. Aharonov–Bohm model and higher degree Levinson theorem

In this section, we first introduce the Aharonov–Bohm model, and discuss some of the results obtained in [41]. In order to extend the discussion about index theorems to index theorems for families, we then provide some information on cyclic cohomology and explain how it can be applied to this model. This material mainly is borrowed from [29] to which we refer for more information.

8.1. The Aharonov–Bohm model

Let us denote by $\mathcal{H}$ the Hilbert space $\mathsf{L}^2(\mathbb{R}^2)$. For any $\alpha \in (0,1)$, we define the vector potential $A_\alpha : \mathbb{R}^2 \setminus \{0\} \to \mathbb{R}^2$ by

$$A_\alpha(x,y) = -\alpha\left(\frac{-y}{x^2+y^2}, \frac{x}{x^2+y^2}\right),$$

which formally corresponds to the magnetic field $B = \alpha\delta$ (δ is the Dirac delta function), and consider the operator

$$H_\alpha := (-i\nabla - A_\alpha)^2, \qquad \mathcal{D}(H_\alpha) = C_c^\infty\big(\mathbb{R}^2 \setminus \{0\}\big) .$$

The closure of this operator in $\mathcal{H}$, which is denoted by the same symbol, is symmetric and has deficiency indices $(2, 2)$.

We briefly recall the parametrization of the self-adjoint extensions of H_α from [41]. Some elements of the domain of the adjoint operator H_α^* admit singularities at the origin. For dealing with them, one defines four linear functionals Φ_0, Φ_{-1}, Ψ_0, Ψ_{-1} on $\mathcal{D}(H_\alpha^*)$ such that for $f \in \mathcal{D}(H_\alpha^*)$ one has, with $\theta \in [0, 2\pi)$ and $r \to 0_+$,

$$2\pi f(r\cos\theta, r\sin\theta) = \Phi_0(f)r^{-\alpha} + \Psi_0(f)r^{\alpha} + e^{-i\theta}\Big(\Phi_{-1}(f)r^{\alpha-1} + \Psi_{-1}(f)r^{1-\alpha}\Big) + O(r).$$

The family of all self-adjoint extensions of the operator H_α is then indexed by two matrices $C, D \in \mathcal{M}_2(\mathbb{C})$ which satisfy the following conditions:

$$\text{(i) } CD^* \text{ is self-adjoint}, \qquad \text{(ii) } \det(CC^* + DD^*) \neq 0, \tag{8.1}$$

and the corresponding extensions H_α^{CD} are the restrictions of H_α^* to the functions f satisfying the boundary conditions

$$C \begin{pmatrix} \Phi_0(f) \\ \Phi_{-1}(f) \end{pmatrix} = 2D \begin{pmatrix} \alpha\Psi_0(f) \\ (1-\alpha)\Psi_{-1}(f) \end{pmatrix} .$$

For simplicity, we call *admissible* a pair of matrices (C, D) satisfying the conditions mentioned in (8.1).

Remark 8.1. The parametrization of the self-adjoint extensions of H_α with all admissible pairs (C, D) is very convenient but non-unique. At a certain point, it will be useful to have a one-to-one parametrization of all self-adjoint extensions. So, let us consider $\mathcal{U}_2(\mathbb{C})$ (the group of unitary 2×2 matrices) and set

$$C(U) := \tfrac{1}{2}(1 - U) \quad \text{and} \quad D(U) = \tfrac{i}{2}(1 + U).$$

It is easy to check that $C(U)$ and $D(U)$ satisfy both conditions (8.1). In addition, two different elements U, U' of $\mathcal{U}_2(\mathbb{C})$ lead to two different self-adjoint operators $H_\alpha^{C(U)\,D(U)}$ and $H_\alpha^{C(U')\,D(U')}$, *cf.* [21]. Thus, without ambiguity we can write H_α^U for the operator $H_\alpha^{C(U)\,D(U)}$. Moreover, the set $\{H_\alpha^U \mid U \in \mathcal{U}_2(\mathbb{C})\}$ describes all self-adjoint extensions of H_α. Let us also mention that the normalization of the above maps has been chosen such that $H_\alpha^{-1} \equiv H_\alpha^{10} = H_\alpha^{AB}$ which corresponds to the standard Aharonov–Bohm operator studied in [1, 51].

For the spectral theory, let us mention that the essential spectrum of H_α^{CD} is absolutely continuous and covers the positive half-line $[0, +\infty)$. On the other hand, the discrete spectrum consists in at most two negative eigenvalues. More precisely, the number of negative eigenvalues of H_α^{CD} coincides with the number of negative eigenvalues of the matrix CD^*.

8.1.1. Wave and scattering operators. One of the main results of [41] is an explicit description of the wave operators. We shall recall this result below, but we first need to introduce the decomposition of the Hilbert space $\mathcal{H}$ with respect to a special basis. For any $m \in \mathbb{Z}$, let ϕ_m be the complex function defined by $[0, 2\pi) \ni \theta \mapsto \phi_m(\theta) := \frac{e^{im\theta}}{\sqrt{2\pi}}$. One has then the canonical isomorphism

$$\mathcal{H} \cong \bigoplus_{m\in\mathbb{Z}} \mathcal{H}_r \otimes [\phi_m] \ , \tag{8.2}$$

where $\mathcal{H}_r := \mathsf{L}^2(\mathbb{R}_+, r\,\mathrm{d}r)$ and $[\phi_m]$ denotes the one-dimensional space spanned by ϕ_m. For shortness, we write $\mathcal{H}_m$ for $\mathcal{H}_r \otimes [\phi_m]$, and often consider it as a subspace of $\mathcal{H}$. Let us still set

$$\mathcal{H}_{\mathtt{int}} := \mathcal{H}_0 \oplus \mathcal{H}_{-1} \tag{8.3}$$

which is clearly isomorphic to $\mathcal{H}_r \otimes \mathbb{C}^2$.

Let us also recall that the unitary dilation group $\{U_t\}_{t\in\mathbb{R}}$ in $\mathcal{H}$ is defined on any $f \in \mathcal{H}$ and $x \in \mathbb{R}^2$ by $[U_t f](x) = e^t f(e^t x)$. Its self-adjoint generator is still denoted by A. It is easily observed that this group as well as its generator leave each subspace $\mathcal{H}_m$ invariant.

Let us now consider the wave operators

$$W_-^{CD} \equiv W_-(H_\alpha^{CD}, H_0) := s - \lim_{t\to-\infty} e^{itH_\alpha^{CD}}\, e^{-itH_0} \ ,$$

where $H_0 := -\Delta$ denotes the Laplace operator on $\mathbb{R}^2$. It is well known that for any admissible pair (C, D) the operator W_-^{CD} is reduced by the decomposition $\mathcal{H} = \mathcal{H}_{\mathtt{int}} \oplus \mathcal{H}_{\mathtt{int}}^\perp$ and that $W_-^{CD}|_{\mathcal{H}_{\mathtt{int}}^\perp} = W_-^{AB}|_{\mathcal{H}_{\mathtt{int}}^\perp}$. The restriction to $\mathcal{H}_{\mathtt{int}}^\perp$ is further reduced by the decomposition (8.2) and it is proved in [41, Prop. 11] that the channel wave operators satisfy for each $m \in \mathbb{Z}$,

$$W_{-,m}^{AB} = \varphi_m^-(A) \ ,$$

with φ_m^- explicitly given for $x \in \mathbb{R}$ by

$$\varphi_m^-(x) := e^{i\delta_m^\alpha}\, \frac{\Gamma\big(\frac{1}{2}(|m|+1+ix)\big)}{\Gamma\big(\frac{1}{2}(|m|+1-ix)\big)}\, \frac{\Gamma\big(\frac{1}{2}(|m+\alpha|+1-ix)\big)}{\Gamma\big(\frac{1}{2}(|m+\alpha|+1+ix)\big)}$$

and

$$\delta_m^\alpha = \tfrac{1}{2}\pi\big(|m| - |m+\alpha|\big) = \begin{cases} -\frac{1}{2}\pi\alpha & \text{if } \ m \geq 0 \\ \ \ \frac{1}{2}\pi\alpha & \text{if } \ m < 0 \end{cases} .$$

Note that here, Γ corresponds to the usual Gamma function. It is also proved in [41, Thm. 12] that

$$W_-^{CD}|_{\mathcal{H}_{\mathtt{int}}} = \begin{pmatrix} \varphi_0^-(A) & 0 \\ 0 & \varphi_{-1}^-(A) \end{pmatrix} + \begin{pmatrix} \tilde{\varphi}_0(A) & 0 \\ 0 & \tilde{\varphi}_{-1}(A) \end{pmatrix} \widetilde{S}_\alpha^{CD}(\sqrt{H_0})$$

with $\tilde{\varphi}_m(x)$ given for $m \in \{0, -1\}$ by

$$\frac{1}{2\pi}\, e^{-i\pi|m|/2}\, e^{\pi x/2}\, \frac{\Gamma\big(\frac{1}{2}(|m|+1+ix)\big)}{\Gamma\big(\frac{1}{2}(|m|+1-ix)\big)} \Gamma\big(\tfrac{1}{2}(1+|m+\alpha|-ix)\big)\,\Gamma\big(\tfrac{1}{2}(1-|m+\alpha|-ix)\big) \ ,$$

and with the function $\widetilde{S}^{CD}_\alpha(\cdot)$ given for $\lambda \in \mathbb{R}_+$ by

$$\begin{aligned}\widetilde{S}^{CD}_\alpha(\lambda) := 2i\sin(\pi\alpha) &\begin{pmatrix} \frac{\Gamma(1-\alpha)\,e^{-i\pi\alpha/2}}{2^\alpha}\,\lambda^\alpha & 0 \\ 0 & \frac{\Gamma(\alpha)\,e^{-i\pi(1-\alpha)/2}}{2^{1-\alpha}}\,\lambda^{(1-\alpha)}\end{pmatrix} \\ &\cdot \left[D\begin{pmatrix} \frac{\Gamma(1-\alpha)^2\,e^{-i\pi\alpha}}{4^\alpha}\,\lambda^{2\alpha} & 0 \\ 0 & \frac{\Gamma(\alpha)^2\,e^{-i\pi(1-\alpha)}}{4^{1-\alpha}}\,\lambda^{2(1-\alpha)}\end{pmatrix} + \frac{\pi}{2\sin(\pi\alpha)}C\right]^{-1} D \\ &\cdot \begin{pmatrix} \frac{\Gamma(1-\alpha)\,e^{-i\pi\alpha/2}}{2^\alpha}\,\lambda^\alpha & 0 \\ 0 & -\frac{\Gamma(\alpha)\,e^{-i\pi(1-\alpha)/2}}{2^{1-\alpha}}\,\lambda^{(1-\alpha)}\end{pmatrix}.\end{aligned}$$

Clearly, the functions φ^-_m and $\tilde{\varphi}_m$ are continuous on $\mathbb{R}$. Furthermore, these functions admit limits at $\pm\infty$: $\varphi^-_m(-\infty) = 1$, $\varphi^-_m(+\infty) = e^{2i\delta^\alpha_m}$, $\tilde{\varphi}_m(-\infty) = 0$ and $\tilde{\varphi}_m(+\infty) = 1$. On the other hand, the relation between the usual scattering operator $S^{CD}_\alpha := \big(W^{CD}_+\big)^* W^{CD}_-$ and the function $\widetilde{S}^{CD}_\alpha(\cdot)$ is provided by the formulas

$$S^{CD}_\alpha|_{\mathcal{H}_{\rm int}} = S^{CD}_\alpha(\sqrt{H_0}) \quad \text{with} \quad S^{CD}_\alpha(\lambda) := \begin{pmatrix} e^{-i\pi\alpha} & 0 \\ 0 & e^{i\pi\alpha}\end{pmatrix} + \widetilde{S}^{CD}_\alpha(\lambda)\ .$$

Let us now state a result which has been formulated in a more precise form in [41, Prop. 14].

Proposition 8.2. *The map*

$$\mathbb{R}_+ \ni \lambda \mapsto S^{CD}_\alpha(\lambda) \in \mathcal{U}_2(\mathbb{C})$$

is norm continuous and has explicit asymptotic values for $\lambda = 0$ and $\lambda = +\infty$ which depend on C, D and α.

The asymptotic values $S^{CD}_\alpha(0)$ and $S^{CD}_\alpha(+\infty)$ are explicitly provided in the statement of [41, Prop. 14], but numerous cases have to be considered. For simplicity, we do not provide these details here. By summarizing the information obtained so far, one infers that:

Theorem 8.3. *For any admissible pair (C, D) the following equality holds:*

$$\begin{aligned}W^{CD}_-|_{\mathcal{H}_{\rm int}} = &\begin{pmatrix}\varphi^-_0(A) & 0 \\ 0 & \varphi^-_{-1}(A)\end{pmatrix} \\ &+ \begin{pmatrix}\tilde{\varphi}_0(A) & 0 \\ 0 & \tilde{\varphi}_{-1}(A)\end{pmatrix}\left[S^{CD}_\alpha(\sqrt{H_0}) - \begin{pmatrix} e^{-i\pi\alpha} & 0 \\ 0 & e^{i\pi\alpha}\end{pmatrix}\right],\end{aligned} \tag{8.4}$$

with $\varphi^-_0, \varphi^-_1, \tilde{\varphi}_0, \tilde{\varphi}_1 \in C([-\infty, \infty])$ and with $S^{CD}_\alpha \in C([0, +\infty])$.

Based on this result and on the content of Section 4, one could easily deduce an index type theorem. However, we prefer to come back to an *ad hoc* approach, which looks more like the approach followed for the baby model. Its interest is that individual contributions to the winding number can be computed, and the importance of each of them is thus emphasized. A more conceptual (and shorter) proof will be provided in Section 8.5.

8.2. Levinson's theorem, the pedestrian approach

Let us start by considering again the expression (8.4) for the operator $W_-^{CD}|_{\mathcal{H}_{\rm int}}$. Since the matrix-valued functions defining this operator have limits at $-\infty$ and $+\infty$, respectively at 0 and $+\infty$, one can define the quadruple $(\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4)$, with Γ_j given for $x \in \mathbb{R}$ and $\lambda \in \mathbb{R}_+$ by

$$
\begin{aligned}
\Gamma_1(x) \equiv \Gamma_1(C,D,\alpha,x) &:= \begin{pmatrix} \varphi_0^-(x) & 0 \\ 0 & \varphi_{-1}^-(x) \end{pmatrix} + \begin{pmatrix} \tilde{\varphi}_0(x) & 0 \\ 0 & \tilde{\varphi}_{-1}(x) \end{pmatrix} \widetilde{S}_\alpha^{CD}(0) \ , \\
\Gamma_2(\lambda) \equiv \Gamma_2(C,D,\alpha,\lambda) &:= S_\alpha^{CD}(\lambda) \ , \qquad (8.5) \\
\Gamma_3(x) \equiv \Gamma_3(C,D,\alpha,x) &:= \begin{pmatrix} \varphi_0^-(x) & 0 \\ 0 & \varphi_{-1}^-(x) \end{pmatrix} + \begin{pmatrix} \tilde{\varphi}_0(x) & 0 \\ 0 & \tilde{\varphi}_{-1}(x) \end{pmatrix} \widetilde{S}_\alpha^{CD}(+\infty) \ , \\
\Gamma_4(\lambda) \equiv \Gamma_4(C,D,\alpha,\lambda) &:= 1.
\end{aligned}
$$

Clearly, $\Gamma_1(\cdot)$ and $\Gamma_3(\cdot)$ are continuous functions on $[-\infty,\infty]$ with values in $\mathcal{U}_2(\mathbb{C})$, and $\Gamma_2(\cdot)$ and $\Gamma_4(\cdot)$ are continuous functions on $[0,\infty]$ with values in $\mathcal{U}_2(\mathbb{C})$. By mimicking the approach of Section 2, one sets $\square = B_1 \cup B_2 \cup B_3 \cup B_4$ with $B_1 = \{0\} \times [-\infty,+\infty]$, $B_2 = [0,+\infty] \times \{+\infty\}$, $B_3 = \{+\infty\} \times [-\infty,+\infty]$, and $B_4 = [0,+\infty] \times \{-\infty\}$, and observes that the function $\Gamma_\alpha^{CD} = (\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4)$ belongs to $C\big(\square; \mathcal{U}_2(\mathbb{C})\big)$. As a consequence, the winding number $\mathrm{Wind}\big(\Gamma_\alpha^{CD}\big)$ based on the map

$$\square \ni \xi \mapsto \det\big[\Gamma_\alpha^{CD}(\xi)\big] \in \mathbb{T}$$

is well defined, and our aim is to relate it to the spectral properties of H_α^{CD}.

The following statement is our Levinson-type theorem for this model:

Theorem 8.4. *For any $\alpha \in (0,1)$ and any admissible pair (C,D) one has*

$$\mathrm{Wind}\big(\Gamma_\alpha^{CD}\big) = \#\sigma_p(H_\alpha^{CD}).$$

The proof of this equality can be obtained by a case-by-case study. It is a rather long computation which has been performed in [41, Sec. III] and we shall only recall the detailed results. Note that one has to calculate separately the contribution to the winding number from the functions Γ_1, Γ_2 and Γ_3, the contribution of Γ_4 being always trivial. Below, the contribution to the winding of the function Γ_j will be denoted by $w_j(\Gamma_\alpha^{CD})$. Let us also stress that due to (8.5) the contribution of Γ_2 corresponds to the contribution of the scattering operator. It will be rather clear that a naive approach of Levinson's theorem involving only the contribution of the scattering operator would lead to a completely wrong result.

We now list the results for the individual contributions. They clearly depend on α, C and D. The various cases have been divided into subfamilies.

Conditions	$\#\sigma_p(H_\alpha^{CD})$	$w_1(\Gamma_\alpha^{CD})$	$w_2(\Gamma_\alpha^{CD})$	$w_3(\Gamma_\alpha^{CD})$	$\mathrm{Wind}(\Gamma_\alpha^{CD})$
$D = 0$	0	0	0	0	0
$C = 0$	0	-1	0	1	0

Now, if $\det(D) \neq 0$ and $\det(C) \neq 0$, we set $E := D^{-1}C =: (e_{jk})_{j,k=1}^2$ and obtains:

Conditions	$\#\sigma_p(H_\alpha^{CD})$	$w_1(\Gamma_\alpha^{CD})$	$w_2(\Gamma_\alpha^{CD})$	$w_3(\Gamma_\alpha^{CD})$	$\mathrm{Wind}(\Gamma_\alpha^{CD})$
$e_{11}e_{22} \geq 0$, $\mathrm{tr}(E) > 0$, $\det(E) > 0$	0	0	-1	1	0
$e_{11}e_{22} \geq 0$, $\mathrm{tr}(E) > 0$, $\det(E) < 0$	1	0	0	1	1
$e_{11}e_{22} \geq 0$, $\mathrm{tr}(E) < 0$, $\det(E) > 0$	2	0	1	1	2
$e_{11}e_{22} \geq 0$, $\mathrm{tr}(E) < 0$, $\det(E) < 0$	1	0	0	1	1
$e_{11} = e_{22} = 0, \det(E) < 0$	1	0	0	1	1
$e_{11}\, e_{22} < 0$	1	0	0	1	1

If $\det(D) \neq 0$, $\det(C) = 0$ and if we still set $E := D^{-1}C$ one has:

Conditions	$\#\sigma_p(H_\alpha^{CD})$	$w_1(\Gamma_\alpha^{CD})$	$w_2(\Gamma_\alpha^{CD})$	$w_3(\Gamma_\alpha^{CD})$	$\mathrm{Wind}(\Gamma_\alpha^{CD})$
$e_{11} = 0, \mathrm{tr}(E) > 0$	0	$-\alpha$	$\alpha - 1$	1	0
$e_{11}\, e_{22} \neq 0, \mathrm{tr}(E) > 0, \alpha < 1/2$	0	$-\alpha$	$\alpha - 1$	1	0
$e_{11} > 0, \mathrm{tr}(E) < 0$	1	$-\alpha$	α	1	1
$e_{11}\, e_{22} \neq 0, \mathrm{tr}(E) < 0, \alpha < 1/2$	1	$-\alpha$	α	1	1
$e_{22} = 0, \mathrm{tr}(E) > 0$	0	$\alpha - 1$	$-\alpha$	1	0
$e_{11}\, e_{22} \neq 0, \mathrm{tr}(E) > 0, \alpha > 1/2$	0	$\alpha - 1$	$-\alpha$	1	0
$e_{22} = 0, \mathrm{tr}(E) < 0$	1	$\alpha - 1$	$1 - \alpha$	1	1
$e_{11}\, e_{22} \neq 0, \mathrm{tr}(E) < 0, \alpha > 1/2$	1	$\alpha - 1$	$1 - \alpha$	1	1
$e_{11}\, e_{22} \neq 0, \mathrm{tr}(E) > 0, \alpha = 1/2$	0	$-1/2$	$-1/2$	1	0
$e_{11}\, e_{22} \neq 0, \mathrm{tr}(E) < 0, \alpha = 1/2$	1	$-1/2$	$1/2$	1	1

On the other hand, if $\dim[\mathrm{Ker}(D)] = 1$, let us define the identification map $I : \mathbb{C} \to \mathbb{C}^2$ with $\mathrm{Ran}(I) = \mathrm{Ker}(D)^\perp$. We then set

$$\ell := (DI)^{-1}CI : \mathbb{C} \to \mathbb{C} \tag{8.6}$$

which is in fact a real number because of the condition of admissibility for the pair (C, D).

In the special case $\alpha = 1/2$ one has:

Conditions	$\#\sigma_p(H_\alpha^{CD})$	$w_1(\Gamma_\alpha^{CD})$	$w_2(\Gamma_\alpha^{CD})$	$w_3(\Gamma_\alpha^{CD})$	$\mathrm{Wind}(\Gamma_\alpha^{CD})$
$\ell > 0$	0	0	$-1/2$	$1/2$	0
$\ell = 0$	0	$-1/2$	0	$1/2$	0
$\ell < 0$	1	0	$1/2$	$1/2$	1

If $\dim[\mathrm{Ker}(D)] = 1$, $\alpha < 1/2$ and if ${}^t(p_1, p_2) \in \mathrm{Ker}(D)$ with $p_1^2 + p_2^2 = 1$ one obtains with ℓ defined in (8.6):

Conditions	$\#\sigma_p(H_\alpha^{CD})$	$w_1(\Gamma_\alpha^{CD})$	$w_2(\Gamma_\alpha^{CD})$	$w_3(\Gamma_\alpha^{CD})$	$\mathrm{Wind}(\Gamma_\alpha^{CD})$
$\ell < 0, p_1 \neq 0$	1	0	α	$1-\alpha$	1
$\ell < 0, p_1 = 0$	1	0	$1-\alpha$	α	1
$\ell > 0, p_1 \neq 0$	0	0	$\alpha-1$	$1-\alpha$	0
$\ell > 0, p_1 = 0$	0	0	$-\alpha$	α	0
$\ell = 0, p_1 p_2 \neq 0$	0	$-\alpha$	$2\alpha-1$	$1-\alpha$	0
$\ell = 0, p_1 = 0$	0	$-\alpha$	0	α	0
$\ell = 0, p_2 = 0$	0	$\alpha-1$	0	$1-\alpha$	0

Finally, if $\dim[\mathrm{Ker}(D)] = 1$, $\alpha > 1/2$ and ${}^t(p_1, p_2) \in \mathrm{Ker}(D)$ with $p_1^2 + p_2^2 = 1$ one has with ℓ defined in (8.6):

Conditions	$\#\sigma_p(H_\alpha^{CD})$	$w_1(\Gamma_\alpha^{CD})$	$w_2(\Gamma_\alpha^{CD})$	$w_3(\Gamma_\alpha^{CD})$	$\mathrm{Wind}(\Gamma_\alpha^{CD})$
$\ell < 0, p_2 \neq 0$	1	0	$1-\alpha$	α	1
$\ell < 0, p_2 = 0$	1	0	α	$1-\alpha$	1
$\ell > 0, p_2 \neq 0$	0	0	$-\alpha$	α	0
$\ell > 0, p_2 = 0$	0	0	$\alpha-1$	$1-\alpha$	0
$\ell = 0, p_1 p_2 \neq 0$	0	$\alpha-1$	$1-2\alpha$	α	0
$\ell = 0, p_1 = 0$	0	$-\alpha$	0	α	0
$\ell = 0, p_2 = 0$	0	$\alpha-1$	0	$1-\alpha$	0

Once again, by looking at these tables, it clearly appears that singling out the contribution due to the scattering operator has no meaning. An index theorem can be obtained only if the three contributions are considered on an equal footing.

8.3. Cyclic cohomology, n-traces and Connes' pairing

In this section we extend the framework which led to our abstract Levinson theorem, namely to Theorem 4.4. In fact, this statement can then be seen as a special case of a more general result. For this part of the manuscript, we refer to [29] and [12, Sec. III], or to the short surveys presented in [33, Sec. 5] and in [34, Sec. 4 and 5].

Given a complex algebra $\mathcal{B}$ and any $n \in \mathbb{N} \cup \{0\}$, let $C^n_\lambda(\mathcal{B})$ be the set of $(n+1)$-linear functional on $\mathcal{B}$ which are cyclic in the sense that any $\eta \in C^n_\lambda(\mathcal{B})$ satisfies for each $w_0, \dots, w_n \in \mathcal{B}$:

$$\eta(w_1, \dots, w_n, w_0) = (-1)^n \eta(w_0, \dots, w_n) \ .$$

Then, let $\mathtt{b} : C^n_\lambda(\mathcal{B}) \to C^{n+1}_\lambda(\mathcal{B})$ be the Hochschild coboundary map defined for $w_0, \dots, w_{n+1} \in \mathcal{B}$ by

$$[\mathtt{b}\eta](w_0, \dots, w_{n+1}) := \sum_{j=0}^{n} (-1)^j \eta(w_0, \dots, w_j w_{j+1}, \dots, w_{n+1}) + (-1)^{n+1} \eta(w_{n+1} w_0, \dots, w_n) \ .$$

An element $\eta \in C^n_\lambda(\mathcal{B})$ satisfying $\mathtt{b}\eta = 0$ is called a cyclic n-cocyle, and the cyclic cohomology $HC(\mathcal{B})$ of $\mathcal{B}$ is the cohomology of the complex

$$0 \to C^0_\lambda(\mathcal{B}) \to \cdots \to C^n_\lambda(\mathcal{B}) \xrightarrow{\mathtt{b}} C^{n+1}_\lambda(\mathcal{B}) \to \dots \ .$$

A convenient way of looking at cyclic n-cocycles is in terms of characters of a graded differential algebra over $\mathcal{B}$. So, let us first recall that a graded differential algebra $(\mathcal{A}, \mathtt{d})$ is a graded algebra $\mathcal{A}$ together with a map $\mathtt{d} : \mathcal{A} \to \mathcal{A}$ of degree $+1$. More precisely, $\mathcal{A} := \oplus_{j=0}^\infty \mathcal{A}_j$ with each $\mathcal{A}_j$ an algebra over $\mathbb{C}$ satisfying the property $\mathcal{A}_j \, \mathcal{A}_k \subset \mathcal{A}_{j+k}$, and $\mathtt{d}$ is a graded derivation satisfying $\mathtt{d}^2 = 0$. In particular, the derivation satisfies $\mathtt{d}(w_1 w_2) = (\mathtt{d}w_1) w_2 + (-1)^{\deg(w_1)} w_1 (\mathtt{d}w_2)$, where $\deg(w_1)$ denotes the degree of the homogeneous element w_1.

A cycle $(\mathcal{A}, \mathtt{d}, \int)$ of dimension n is a graded differential algebra $(\mathcal{A}, \mathtt{d})$, with $\mathcal{A}_j = 0$ for $j > n$, endowed with a linear functional $\int : \mathcal{A}_n \to \mathbb{C}$ satisfying $\int \mathtt{d}w = 0$ if $w \in \mathcal{A}_{n-1}$, and for $w_j \in \mathcal{A}_j$, $w_k \in \mathcal{A}_k$ with $j + k = n$:

$$\int w_j w_k = (-1)^{jk} \int w_k w_j \ .$$

Given an algebra $\mathcal{B}$, a cycle of dimension n over $\mathcal{B}$ is a cycle $(\mathcal{A}, \mathtt{d}, \int)$ of dimension n together with a homomorphism $\rho : \mathcal{B} \to \mathcal{A}_0$. In the sequel, we will assume that this map is injective and hence identify $\mathcal{B}$ with a subalgebra of $\mathcal{A}_0$ (and do not write ρ anymore). Now, if $w_0, \dots, w_n$ are $n+1$ elements of $\mathcal{B}$, one can define the character $\eta(w_0, \dots, w_n) \in \mathbb{C}$ by the formula:

$$\eta(w_0, \dots, w_n) := \int w_0 \, (\mathtt{d}w_1) \dots (\mathtt{d}w_n) \ . \tag{8.7}$$

As shown in [12, Prop. III.1.4], the map $\eta : \mathcal{B}^{n+1} \to \mathbb{C}$ is a cyclic $(n+1)$-linear functional on $\mathcal{B}$ satisfying $\mathtt{b}\eta = 0$, *i.e.*, η is a cyclic n-cocycle. Conversely, any cyclic n-cocycle arises as the character of a cycle of dimension n over $\mathcal{B}$. Let us also mention that a third description of any cyclic n-cocycle is presented in [12, Sec. III.1.α] in terms of the universal graded differential algebra associated with $\mathcal{B}$.

We can now introduce the precise definition of a n-trace over a Banach algebra. Recall that for an algebra $\mathcal{B}$ that is not necessarily unital, we denote by $\mathcal{B}^+$ the canonical algebra obtained by adding a unit to $\mathcal{B}$.

Definition 8.5. A n-trace on a Banach algebra $\mathcal{B}$ is the character of a cycle $(\mathcal{A}, \mathtt{d}, \int)$ of dimension n over a dense subalgebra $\mathcal{B}'$ of $\mathcal{B}$ such that for all $w_1, \dots, w_n \in \mathcal{B}'$ and any $x_1, \dots, x_n \in (\mathcal{B}')^+$ there exists a constant $c = c(w_1, \dots, w_n)$ such that

$$\left| \int (x_1 \mathtt{d} w_1) \dots (x_n \mathtt{d} w_n) \right| \leq c \|x_1\| \dots \|x_n\| \ .$$

Remark 8.6. Typically, the elements of $\mathcal{B}'$ are suitably smooth elements of $\mathcal{B}$ on which the derivation $\mathtt{d}$ is well defined and for which the r.h.s. of (8.7) is also well defined. However, the action of the n-trace η can sometimes be extended to more general elements $(w_0, \dots, w_n) \in \mathcal{B}^{n+1}$ by a suitable reinterpretation of the l.h.s. of (8.7).

The importance of n-traces relies on their duality relation with K-groups. Recall first that $\mathcal{M}_q(\mathcal{B}) \cong \mathcal{B} \otimes \mathcal{M}_q(\mathbb{C})$ and that tr denotes the standard trace on matrices. Now, let $\mathcal{B}$ be a C^*-algebra and let η_n be a n-trace on $\mathcal{B}$ with $n \in \mathbb{N}$ even. If $\mathcal{B}'$ is the dense subalgebra of $\mathcal{B}$ mentioned in Definition 8.5 and if p is a projection in $\mathcal{M}_q(\mathcal{B}')$, then one sets

$$\langle \eta_n, p \rangle := c_n \, [\eta_n \# \mathrm{tr}](p, \dots, p),$$

where $\#$ denotes the cup product. Similarly, if $\mathcal{B}$ is a unital C^*-algebra and if η_n is a normalized n-trace with $n \in \mathbb{N}$ odd, then for any unitary u in $\mathcal{M}_q(\mathcal{B}')$ one sets

$$\langle \eta_n, u \rangle := c_n \, [\eta_n \# \mathrm{tr}](u^*, u, u^*, \dots, u)$$

the entries on the r.h.s. alternating between u and u^*. The constants c_n are given by

$$c_{2k} = \frac{1}{(2\pi i)^k} \frac{1}{k!} \ , \qquad c_{2k-1} = \frac{1}{(2\pi i)^k} \frac{1}{2^{2k+1}} \frac{1}{(k - \frac{1}{2}) \cdots \frac{1}{2}} \ . \tag{8.8}$$

These relations are referred to as Connes' pairing between K-theory and cyclic cohomology of $\mathcal{B}$ because of the following property, see [12, Sec. III] for precise statements and for the proofs: In the above framework, the values $\langle \eta_n, p \rangle$ and $\langle \eta_n, u \rangle$ depend only on the K_0-class $[p]_0$ of p and on the K_1-class $[u]_1$ of u, respectively.

We now illustrate these notions by revisiting Example 4.1.

Example 8.7. If $\mathcal{B} = \mathcal{K}(\mathcal{H})$, the algebra of compact operators on a Hilbert space $\mathcal{H}$, then the linear functional $\int$ on $\mathcal{B}$ is given by the usual trace Tr on the set $\mathcal{K}_1(\mathcal{H})$ of trace class elements of $\mathcal{K}(\mathcal{H})$. Furthermore, since any projection $p \in \mathcal{K}(\mathcal{H})$ is trace class, it follows that $\langle \eta_0, p \rangle \equiv \langle \mathrm{Tr}, p \rangle$ is well defined for any such p and that this expression gives the dimension of the projection p.

For the next example, let us recall that det denotes the usual determinant of elements of $\mathcal{M}_q(\mathbb{C})$.

Example 8.8. If $\mathcal{B} = C(\mathbb{S}, \mathbb{C})$, let us fix $\mathcal{B}' := C^1(\mathbb{S}, \mathbb{C})$. We parameterize $\mathbb{S}$ by the real numbers modulo 2π using θ as local coordinate. As usual, for any $w \in \mathcal{B}'$ (which corresponds to a homogeneous element of degree 0), one sets $[\mathtt{d}w](\theta) := w'(\theta)\,\mathrm{d}\theta$ (which is now a homogeneous element of degree 1). Furthermore, we define the graded trace $\int v\,\mathrm{d}\theta := \int_0^{2\pi} v(\theta)\,\mathrm{d}\theta$ for an arbitrary element $v\,\mathrm{d}\theta$ of degree 1. This defines the 1-trace η_1. A unitary element in $u \in C^1\big(\mathbb{S}, \mathcal{M}_q(\mathbb{C})\big) \equiv \mathcal{M}_q\big(C^1(\mathbb{S}; \mathbb{C})\big)$ pairs as follows

$$\begin{aligned}\langle \eta_1, u\rangle = c_1[\eta_1 \# \mathrm{tr}](u^*, u) &:= \frac{1}{2\pi i}\int_0^{2\pi} \mathrm{tr}[u(\theta)^*\, u'(\theta)]\,\mathrm{d}\theta \\ &= -\frac{1}{2\pi}\int_0^{2\pi} \mathrm{tr}[iu(\theta)^*\, u'(\theta)]\,\mathrm{d}\theta\ . \end{aligned} \tag{8.9}$$

But this quantity has already been encountered at several places in this text and corresponds to analytic expression for the computation of (minus)[8] the winding number of the map $\theta \mapsto \det[u(\theta)]$. Since this quantity is of topological nature, it only requires that the map $\theta \mapsto u(\theta)$ is continuous. Altogether, one has thus obtained that the pairing $\langle \eta_1, u\rangle$ in (8.9) is nothing but the computation of (minus) the winding number of the map $\det[u] : \mathbb{S} \to \mathbb{T}$, valid for any unitary $u \in C\big(\mathbb{S}, \mathcal{M}_q(\mathbb{C})\big)$. In other words, one has obtained that $\langle \eta_1, u\rangle = -\mathrm{Wind}(u)$.

8.4. Dual boundary maps

We have seen that an n-trace η over $\mathcal{B}$ gives rise to a functional on $K_i(\mathcal{B})$ for $i = 0$ or $i = 1$, *i.e.*, the map $\langle \eta, \cdot\rangle$ is an element of $\mathrm{Hom}\,(K_i(\mathcal{B}), \mathbb{C})$. In that sense n-traces are dual to the elements of the K-groups. An important question is whether this dual relation is functorial in the sense that morphisms between the K-groups of different algebras yield dual morphisms on higher traces. Here we are in particular interested in a map on higher traces which is dual to the index map, *i.e.*, a map # which assigns to an even trace η an odd trace $\#\eta$ such that

$$\langle \eta, \mathrm{ind}(\cdot)\rangle = \langle \#\eta, \cdot\rangle. \tag{8.10}$$

This situation gives rise to equalities between two numerical topological invariants.

Such an approach for relating two topological invariants has already been used at few occasions. For example, our abstract Levinson theorem (Theorem 4.4) corresponds to a equality of the form (8.10) for a 0-trace and a 1-trace. In addition, in the following section we shall develop such an equality for a 2-trace and a 3-trace. On the other hand, let us mention that similar equalities have also been developed for the exponential map in (8.10) instead of the index map. In this framework, an equality involving a 0-trace and a 1-trace has been put into

[8]Unfortunately, due to our convention for the computation of the winding number, the expressions computed with the constants provided in (8.8) differ from our expressions by a minus sign.

evidence in [28]. It gives rise to a relation between the pressure on the boundary of a quantum system and the integrated density of states. Similarly, a relation involving 2-trace and a 1-trace was involved in the proof of the equality between the bulk-Hall conductivity and the conductivity of the current along the edge of the sample, see [33, 34].

8.5. Higher degree Levinson theorem

In order to derive a higher degree Levinson theorem, let us first introduce the algebraic framework which will lead to a much shorter new proof of Theorem 8.4. The construction is similar to the one already proposed in Section 6.2 for Schrödinger operators on $\mathbb{R}^3$.

We recall from Section 8.1 that $\mathcal{H}$ denotes the Hilbert space $\mathsf{L}^2(\mathbb{R}^2)$, that $\mathcal{H}_{\mathtt{int}}$ has been introduced in (8.3), and let us set $\mathfrak{h} := \mathsf{L}^2(\mathbb{S})$. We also denote by $\mathscr{F}_0 : \mathcal{H} \mapsto \mathsf{L}^2(\mathbb{R}_+;\mathfrak{h})$ the usual spectral representation of the Laplace operator $H_0 = -\Delta$ in $\mathcal{H}$. Then, we can define

$$\mathcal{E} := \big\{\mathscr{F}_0^*\big[\mathcal{E}_{(L,A)} \otimes \mathcal{K}(\mathfrak{h})\big]\mathscr{F}_0\big\}|_{\mathcal{H}_{\mathtt{int}}} \subset \mathcal{B}\big(\mathcal{H}_{\mathtt{int}}\big) \equiv \mathcal{B}(\mathcal{H}_r) \otimes \mathcal{M}_2(\mathbb{C}).$$

Clearly, $\mathcal{E}$ is made of continuous functions of H_0 having limits at 0 and $+\infty$, and of continuous function of the generator A of dilations in $\mathsf{L}^2(\mathbb{R}^2)$ having limits at $-\infty$ and at $+\infty$. One can then consider the short exact sequence

$$0 \to \mathcal{K}(\mathcal{H}_{\mathtt{int}}) \hookrightarrow \mathcal{E} \xrightarrow{q} C\big(\square;\mathcal{M}_2(\mathbb{C})\big) \to 0,$$

and infer the following result directly from the construction presented in Section 4. Note that this result corresponds to [29, Thm. 13] and provides an alternative proof for Theorem 8.4.

Theorem 8.9. *For any $\alpha \in (0,1)$ and any admissible pair (C,D), one has*

$$W_-^{CD}|_{\mathcal{H}_{\mathtt{int}}} \in \mathcal{E}.$$

Furthermore, $q\big(W_-^{CD}|_{\mathcal{H}_{\mathtt{int}}}\big) = \Gamma_\alpha^{CD} \in C\big(\square;\mathcal{U}_2(\mathbb{C})\big)$ and the following equality holds

$$\mathrm{Wind}\big(\Gamma_\alpha^{CD}\big) = \#\sigma_p(H_\alpha^{CD}).$$

Let us stress that the previous statement corresponds to a pointwise Levinson theorem in the sense that it has been obtained for fixed C, D and α. However, it clearly calls for making these parameters degrees of freedom and thus to include them into the description of the algebras. In the context of our physical model this amounts to considering families of self-adjoint extensions of H_α. For that purpose we use the one-to-one parametrization of these extensions with elements $U \in \mathcal{U}_2(\mathbb{C})$ introduced in Remark 8.1. We denote the self-adjoint extension corresponding to $U \in \mathcal{U}_2(\mathbb{C})$ by H_α^U.

So, let us consider a smooth and compact orientable n-dimensional manifold $\mathcal{X}$ without boundary. Subsequently, we will choose for $\mathcal{X}$ a two-dimensional submanifold of $\mathcal{U}_2(\mathbb{C}) \times (0,1)$. Taking continuous functions over $\mathcal{X}$ we get a new short exact sequence

$$0 \to C\big(\mathcal{X};\mathcal{K}(\mathcal{H}_{\mathtt{int}})\big) \hookrightarrow C(\mathcal{X};\mathcal{E}) \to C\big(\mathcal{X};C\big(\square;\mathcal{M}_2(\mathbb{C})\big)\big) \to 0\ . \tag{8.11}$$

Furthermore, recall that $\mathcal{K}(\mathcal{H}_{\mathtt{int}})$ is endowed with a 0-trace Tr and the algebra $C\big(\square;\mathcal{M}_2(\mathbb{C})\big)$ with a 1-trace Wind. There is a standard construction in cyclic cohomology, the cup product, which provides us with a suitable n-trace on the algebra $C\big(\mathcal{X},\mathcal{K}(\mathcal{H}_{\mathtt{int}})\big)$ and a corresponding $(n+1)$-trace on the algebra

$$C\big(\mathcal{X};C\big(\square;\mathcal{M}_2(\mathbb{C})\big)\big),$$

see [12, Sec. III.1.α]. We describe it here in terms of cycles.

Recall that any smooth and compact manifold $\mathcal{Y}$ of dimension d naturally defines a structure of a graded differential algebra $(\mathcal{A}_\mathcal{Y},\mathtt{d}_\mathcal{Y})$, the algebra of its smooth differential k-forms. If we assume in addition that $\mathcal{Y}$ is orientable so that we can choose a global volume form, then the linear form $\int_\mathcal{Y}$ can be defined by integrating the d-forms over $\mathcal{Y}$. In that case, the algebra $C(\mathcal{Y})$ is naturally endowed with the d-trace defined by the character of the cycle $(\mathcal{A}_\mathcal{Y},\mathtt{d}_\mathcal{Y},\int_\mathcal{Y})$ of dimension d over the dense subalgebra $C^\infty(\mathcal{Y})$.

For the algebra $C\big(\mathcal{X};\mathcal{K}(\mathcal{H}_{\mathtt{int}})\big)$, let us denote by $\mathcal{K}_1(\mathcal{H}_{\mathtt{int}})$ the trace class elements of $\mathcal{K}(\mathcal{H}_{\mathtt{int}})$. Then, the natural graded differential algebra associated with $C^\infty\big(\mathcal{X},\mathcal{K}_1(\mathcal{H}_{\mathtt{int}})\big)$ is given by $(\mathcal{A}_\mathcal{X}\otimes\mathcal{K}_1(\mathcal{H}_{\mathtt{int}}),\mathtt{d}_\mathcal{X})$.

The resulting n-trace on $C\big(\mathcal{X};\mathcal{K}(\mathcal{H}_{\mathtt{int}})\big)$ is then defined by the character of the cycle $(\mathcal{A}_\mathcal{X}\otimes\mathcal{K}_1(\mathcal{H}_{\mathtt{int}}),\mathtt{d}_\mathcal{X},\int_\mathcal{X}\otimes\mathrm{Tr})$ over the dense subalgebra $C^\infty\big(\mathcal{X},\mathcal{K}_1(\mathcal{H}_{\mathtt{int}})\big)$ of $C\big(\mathcal{X};\mathcal{K}(\mathcal{H}_{\mathtt{int}})\big)$. We denote it by $\eta_\mathcal{X}$.

For the second algebra, let us observe that

$$C\big(\mathcal{X};C\big(\square;\mathcal{M}_2(\mathbb{C})\big)\big)\cong C\big(\mathcal{X}\times\mathbb{S};\mathcal{M}_2(\mathbb{C})\big)\cong C(\mathcal{X}\times\mathbb{S})\otimes\mathcal{M}_2(\mathbb{C}).$$

Since $\mathcal{X}\times\mathbb{S}$ is a compact orientable manifold without boundary, the above construction applies also to $C\big(\mathcal{X}\times\mathbb{S};\mathcal{M}_2(\mathbb{C})\big)$. More precisely, the exterior derivation on $\mathcal{X}\times\mathbb{S}$ is the sum of $\mathtt{d}_\mathcal{X}$ and $\mathtt{d}_\mathbb{S}$ (the latter was denoted simply by $\mathtt{d}$ in Example 8.8). Furthermore, we consider the natural volume form on $\mathcal{X}\times\mathbb{S}$. Note because of the factor $\mathcal{M}_2(\mathbb{C})$ the graded trace of the cycle involves the usual matrix trace tr. Thus the resulting $(n+1)$-trace is the character of the cycle $(\mathcal{A}_{\mathcal{X}\times\mathbb{S}}\otimes\mathcal{M}_2(\mathbb{C}),\mathtt{d}_\mathcal{X}+\mathtt{d}_\mathbb{S},\int_{\mathcal{X}\times\mathbb{S}}\otimes\mathrm{tr})$. We denote it by $\#\eta_\mathcal{X}$.

Having these constructions at our disposal we can now state the main result of this section. For the statement, we use the one-to-one parametrization of the extensions H^U_α of H_α introduced in Remark 8.1. We also consider a family $\{W^{U,\alpha}_-\}_{(U,\alpha)\in\mathcal{X}}\subset\mathcal{B}(\mathcal{H}_{\mathtt{int}})$, with $W^{U,\alpha}_-:=W_-(H^U_\alpha,H_0)$, parameterized by some compact orientable and boundaryless submanifold $\mathcal{X}$ of $\mathcal{U}_2(\mathbb{C})\times(0,1)$. This family defines several maps, namely

$$\mathbf{W}_-:\mathcal{X}\ni(U,\alpha)\mapsto W^{U,\alpha}_-\in\mathcal{E}$$

as well as

$$\mathbf{\Gamma}:\mathcal{X}\ni(U,\alpha)\mapsto\Gamma^{U,\alpha}_\square\in C\big(\square;\mathcal{M}_2(\mathbb{C})\big),$$

with $\Gamma^{U,\alpha}_\square:=q\big(W^{U,\alpha}_-\big)$, and also

$$\mathbf{E}_\mathrm{p}:\mathcal{X}\ni(U,\alpha)\mapsto E_\mathrm{p}\big(H^U_\alpha\big).$$

Theorem 8.10 (Higher degree Levinson theorem). *Let $\mathcal{X}$ be a smooth, compact and orientable n-dimensional submanifold of $\mathcal{U}_2(\mathbb{C}) \times (0,1)$ without boundary. Let us assume that the map $\mathbf{W}_- : \mathcal{X} \to \mathcal{E}$ is continuous. Then the maps $\boldsymbol{\Gamma}$ and $\mathbf{E}_\mathrm{p}$ are continuous, and the following equality holds:*

$$\mathrm{ind}[\boldsymbol{\Gamma}]_1 = -[\mathbf{E}_\mathrm{p}]_0$$

where ind *is the index map from the K_1-group of the algebra $C\big(\mathcal{X}; C\big(\square; \mathcal{M}_2(\mathbb{C})\big)\big)$ to the K_0-group of the algebra $C\big(\mathcal{X}; \mathcal{K}(\mathcal{H}_{\mathsf{int}})\big)$. Furthermore, the numerical equality*

$$\big\langle \#\eta_{\mathcal{X}}, [\boldsymbol{\Gamma}]_1 \big\rangle = -\big\langle \eta_{\mathcal{X}}, [\mathbf{E}_\mathrm{p}]_0 \big\rangle \tag{8.12}$$

also holds.

The proof of this statement is provided in [29, Thm. 15] and is based on the earlier work [33]. Let us point out that r.h.s. of (8.12) corresponds to the Chern number of the vector bundle given by the eigenvectors of H^U_α. On the other hand, the l.h.s. corresponds to a $(n+1)$-trace applied to $\boldsymbol{\Gamma}$ which is constructed from the scattering theory for the operator H^U_α. For these reasons, such an equality has been named *a higher degree Levinson theorem*. In the next section we illustrate this equality by a special choice of the manifold $\mathcal{X}$.

8.5.1. A non-trivial example. Let us now choose a 2-dimensional manifold $\mathcal{X}$ and show that the previous relation between the corresponding 2-trace and 3-trace is not trivial. More precisely, we shall choose a manifold $\mathcal{X}$ such that the r.h.s. of (8.12) is not equal to 0.

For that purpose, let us fix two complex numbers λ_1, λ_2 of modulus 1 with $\mathrm{Im}\lambda_1 < 0 < \mathrm{Im}\lambda_2$ and consider the set $\mathcal{X} \subset \mathcal{U}_2(\mathbb{C})$ defined by:

$$\mathcal{X} = \left\{ V \left(\begin{smallmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{smallmatrix}\right) V^* \mid V \in \mathcal{U}_2(\mathbb{C}) \right\}.$$

Clearly, $\mathcal{X}$ is a two-dimensional smooth and compact manifold without boundary, which can be parameterized by

$$\mathcal{X} = \left\{ \begin{pmatrix} \rho^2\lambda_1 + (1-\rho^2)\lambda_2 & \rho(1-\rho^2)^{1/2}\, e^{i\phi}(\lambda_1 - \lambda_2) \\ \rho(1-\rho^2)^{1/2}\, e^{-i\phi}(\lambda_1 - \lambda_2) & (1-\rho^2)\lambda_1 + \rho^2\lambda_2 \end{pmatrix} \middle| \begin{smallmatrix} \rho \in [0,1] \\ \text{and} \\ \phi \in [0,2\pi) \end{smallmatrix} \right\}. \tag{8.13}$$

Note that the (θ, ϕ)-parametrization of $\mathcal{X}$ is complete in the sense that it covers all the manifold injectively away from a subset of codimension 1, but it has coordinate singularities at $\rho \in \{0, 1\}$.

By [41, Lem. 16], for each $U \equiv U(\rho, \phi) \in \mathcal{X}$ the operator H^U_α has a single negative eigenvalue. It follows that the projection $E_\mathrm{p}(H^U_\alpha)$ is non-trivial for any $\alpha \in (0,1)$ and any $U \in \mathcal{X}$, and thus the expression $\big\langle \eta_{\mathcal{X}}, [\mathbf{E}_\mathrm{p}]_0 \big\rangle$ can be computed. This rather lengthy computation has been performed in [29, Sec. V.D] and it turns out that the following result has been found for this example:

$$\big\langle \eta_{\mathcal{X}}, [\mathbf{E}_\mathrm{p}]_0 \big\rangle = 1.$$

As a corollary of Theorem 8.10 one can then deduce that:

Proposition 8.11. *Let* λ_1, λ_2 *be two complex numbers of modulus* 1 *with* $\mathrm{Im}\lambda_1 < 0 < \mathrm{Im}\lambda_2$ *and consider the set* $\mathcal{X} \subset \mathcal{U}_2(\mathbb{C})$ *defined by* (8.13)*. Then the map* $\mathbf{W}_- : \mathcal{X} \to \mathcal{E}$ *is continuous and the following equality holds:*

$$\frac{1}{24\pi^2}\int_{\mathcal{X}\times\square} \mathrm{tr}\big[\mathbf{\Gamma}^* \,(\mathtt{d}_{\mathcal{X}\times\square}\mathbf{\Gamma}) \wedge (\mathtt{d}_{\mathcal{X}\times\square}\mathbf{\Gamma}^*) \wedge (\mathtt{d}_{\mathcal{X}\times\square}\mathbf{\Gamma})\big] = 1.$$

9. Appendix

9.1. The baby model

In this section, we provide the proofs on the baby model which have not been presented in Section 2. The notations are directly borrowed from this section, but we shall mainly review, modify and extend some results obtained in [57, Sec. 3.1].

First of all, it is shown in [57, Sec. 3.1] that the wave operators $W_\pm^\alpha$ exist and are asymptotically complete. Furthermore, rather explicit expressions for them are proposed in [57, Eq. 3.1.15]. Let us also mention that an expression for the scattering operator S^α is given in [57, Sec. 3.1], namely

$$S^\alpha = \frac{\alpha + i\sqrt{H_{\mathrm{D}}}}{\alpha - i\sqrt{H_{\mathrm{D}}}}.$$

In the following lemma we derive new expressions for the wave operators. They involve the scattering operator S^α as well as the Fourier sine and cosine transforms $\mathscr{F}_{\mathrm{s}}$ and $\mathscr{F}_{\mathrm{c}}$ defined for $x, k \in \mathbb{R}_+$ and any $f \in C_{\mathrm{c}}(\mathbb{R}_+) \subset \mathsf{L}^2(\mathbb{R}_+)$ by

$$[\mathscr{F}_{\mathrm{s}} f](k) := (2/\pi)^{1/2}\int_0^\infty \sin(kx) f(x)\,\mathrm{d}x \tag{9.1}$$

$$[\mathscr{F}_{\mathrm{c}} f](k) := (2/\pi)^{1/2}\int_0^\infty \cos(kx) f(x)\,\mathrm{d}x. \tag{9.2}$$

Lemma 9.1. *The following equalities hold:*

$$W_-^\alpha = 1 + \tfrac{1}{2}\big(1 - i\mathscr{F}_{\mathrm{c}}^*\mathscr{F}_{\mathrm{s}}\big)[S^\alpha - 1],$$
$$W_+^\alpha = 1 + \tfrac{1}{2}\big(1 + i\mathscr{F}_{\mathrm{c}}^*\mathscr{F}_{\mathrm{s}}\big)\big[(S^\alpha)^* - 1\big].$$

Proof. We use the notations of [57, Sec. 3.1] without further explanations. For W_-^α, it follows from [57, Eq. 3.1.15 & 3.1.20] that

$$\begin{aligned} W_-^\alpha &= iP\mathscr{F}_-^*\mathscr{F}_{\mathrm{s}} = \tfrac{i}{2}(2\mathscr{F}_-P)^*\mathscr{F}_{\mathrm{s}} = \tfrac{i}{2}\big(\Pi_+ - S^*\Pi_-\big)^*\mathscr{F}_{\mathrm{s}} \\ &= \tfrac{i}{2}\big(2i\mathscr{F}_{\mathrm{s}} + \Pi_- - S^*\Pi_-\big)^*\mathscr{F}_{\mathrm{s}} = \tfrac{i}{2}\big(-2i\mathscr{F}_{\mathrm{s}}^* - \Pi_-^*(S-1)\big)\mathscr{F}_{\mathrm{s}} \\ &= 1 - \tfrac{i}{2}\Pi_-^*\mathscr{F}_{\mathrm{s}}(S^\alpha - 1). \end{aligned}$$

Thus, one obtains

$$W_-^\alpha = 1 - \tfrac{i}{2}\big(\mathscr{F}_{\mathrm{c}}^* + i\mathscr{F}_{\mathrm{s}}^*\big)\mathscr{F}_{\mathrm{s}}[S^\alpha - 1] = 1 + \tfrac{1}{2}\big(1 - i\mathscr{F}_{\mathrm{c}}^*\mathscr{F}_{\mathrm{s}}\big)[S^\alpha - 1].$$

A similar computation leads to the mentioned result for W_+^α. □

Now, we provide another expression for the operator $-i\mathscr{F}_{\rm c}^*\mathscr{F}_{\rm s}$. For that purpose, let A denote the generator of dilations in $\mathsf{L}^2(\mathbb{R}_+)$.

Lemma 9.2. *The following equality holds*

$$-i\mathscr{F}_{\rm c}^*\mathscr{F}_{\rm s} = \tanh(\pi A) - i\cosh(\pi A)^{-1}.$$

Proof. This proof is inspired by the proof of [31, Lem. 3]. Let us first define for $x, y \in \mathbb{R}_+$ and $\varepsilon > 0$ the kernel of the operator I_ε by

$$I_\varepsilon(x,y) := (1/\pi)\left[\frac{x+y}{(x+y)^2+\varepsilon^2} - \frac{x-y}{(x-y)^2+\varepsilon^2}\right].$$

Then, an easy computation shows that $I_\varepsilon(x,y) = (2/\pi)\int_0^\infty \cos(xz)\sin(yz)\,\mathrm{e}^{-\varepsilon z}\,\mathrm{d}z$, and an application of the theorems of Fubini and Lebesgue for $f \in C_{\rm c}(\mathbb{R}_+)$ leads to the equality

$$\lim_{\varepsilon\searrow 0} I_\varepsilon f = \mathscr{F}_{\rm c}^*\mathscr{F}_{\rm s} f.$$

Now, by comparing the expression for $[I_\varepsilon f](x)$ with the following expression

$$[\varphi(A)f](x) = \frac{1}{\sqrt{2\pi}}\int_0^\infty \check{\varphi}\Big(\ln\big(\frac{x}{y}\big)\Big)\Big(\frac{x}{y}\Big)^{1/2} f(y)\frac{\mathrm{d}y}{x},$$

valid for any essentially bounded function φ on $\mathbb{R}$ whose inverse Fourier transform is a distribution on $\mathbb{R}$, one obtains that

$$\check{\varphi}(s) = \frac{1}{\sqrt{2\pi}}\left[\frac{1}{\cosh(s/2)} - \mathrm{Pv}\frac{1}{\sinh(s/2)}\right],$$

where Pv means principal value. Finally, by using that the Fourier transform of the distribution $s \mapsto \mathrm{Pv}\frac{1}{\sinh(s/2)}$ is the function $-i\sqrt{2\pi}\tanh(\pi\cdot)$ and the one of $s \mapsto \frac{1}{\cosh(s/2)}$ is the function $\sqrt{2\pi}\cosh(\pi\cdot)^{-1}$, one obtains that

$$\varphi(A) = \cosh(\pi A)^{-1} + i\tanh(\pi A).$$

By replacing $\mathscr{F}_{\rm c}^*\mathscr{F}_{\rm s}$ with this expression, one directly obtains the stated result. □

Corollary 9.3. *The following equalities hold:*

$$W_-^\alpha = 1 + \tfrac{1}{2}\big(1 + \tanh(\pi A) - i\cosh(\pi A)^{-1}\big)\left[\frac{\alpha + i\sqrt{H_{\rm D}}}{\alpha - i\sqrt{H_{\rm D}}} - 1\right],$$

$$W_+^\alpha = 1 + \tfrac{1}{2}\big(1 - \tanh(\pi A) + i\cosh(\pi A)^{-1}\big)\left[\frac{\alpha - i\sqrt{H_{\rm D}}}{\alpha + i\sqrt{H_{\rm D}}} - 1\right].$$

9.2. Regularization

Recall that $\mathfrak{h}$ stands for an arbitrary Hilbert space and that $\mathcal{U}(\mathfrak{h})$ corresponds to the set of unitary operators on $\mathfrak{h}$. Let Γ be a map $\mathbb{S} \to \mathcal{U}(\mathfrak{h})$ such that $\Gamma(t) - 1 \in \mathcal{K}(\mathfrak{h})$ for all $t \in \mathbb{S}$. For $p \in \mathbb{N}$ we set $\mathcal{K}_p(\mathfrak{h})$ for the pth Schatten ideal in $\mathcal{K}(\mathfrak{h})$.

Proof of Lemma 6.11. For simplicity, let us set $A(t) := 1 - \Gamma(t)$ for any $t \in I$ and recall from [20, Eq. (XI.2.11)] that $\det_{p+1}\big(\Gamma(t)\big) = \det\big(1 + R_{p+1}(t)\big)$ with

$$R_{p+1}(t) := \Gamma(t) \exp\bigg\{\sum_{j=1}^{p} \frac{1}{j} A(t)^j\bigg\} - 1 \ .$$

Then, for any $t, s \in I$ with $s \neq t$ one has

$$\begin{aligned}\frac{\det_{p+1}\big(\Gamma(s)\big)}{\det_{p+1}\big(\Gamma(t)\big)} = \frac{\det\big(1 + R_{p+1}(s)\big)}{\det\big(1 + R_{p+1}(t)\big)} &= \frac{\det\big[\big(1 + R_{p+1}(t)\big)\big(1 + B_{p+1}(t,s)\big)\big]}{\det\big(1 + R_{p+1}(t)\big)} \\ &= \det\big(1 + B_{p+1}(t,s)\big)\end{aligned}$$

with $B_{p+1}(t,s) = \big(1 + R_{p+1}(t)\big)^{-1}\big(R_{p+1}(s) - R_{p+1}(t)\big)$. Note that $1 + R_{p+1}(t)$ is invertible in $\mathcal{B}(\mathfrak{h})$ because $\det_{p+1}\big(\Gamma(t)\big)$ is non-zero. With these information let us observe that

$$\frac{\frac{\det_{p+1}(\Gamma(s)) - \det_{p+1}(\Gamma(t))}{|s-t|}}{\det_{p+1}(\Gamma(t))} = \frac{1}{|s-t|}\Big[\det\big(1 + B_{p+1}(t,s)\big) - 1\Big] \ . \tag{9.3}$$

Thus, the statement will be obtained if the limit $s \to t$ of this expression exists and if this limit is equal to the r.h.s. of (6.8).

Now, by taking into account the asymptotic development of $\det(1 + \varepsilon X)$ for ε small enough, one obtains that

$$\begin{aligned}\lim_{s\to t} \frac{1}{|s-t|}\Big[\det\big(1 + B_{p+1}(t,s)\big) - 1\Big] &= \lim_{s\to t} \operatorname{tr}\bigg[\frac{B_{p+1}(t,s)}{|s-t|}\bigg] \\ &= \lim_{s\to t} \operatorname{tr}\bigg[H_{p+1}(t)^{-1} \frac{H_{p+1}(s) - H_{p+1}(t)}{|s-t|}\bigg]\end{aligned} \tag{9.4}$$

with $H_{p+1}(t) := \big(1 - A(t)\big) \exp\big\{\sum_{j=1}^{p} \frac{1}{j} A(t)^j\big\}$. Furthermore, it is known that the function h defined for $z \in \mathbb{C}$ by $h(z) := z^{-(p+1)}(1 - z) \exp\big\{\sum_{j=1}^{p} \frac{1}{j} z^j\big\}$ is an entire function, see for example [54, Lem. 6.1]. Thus, from the equality

$$H_{p+1}(t) = A(t)^{p+1} h\big(A(t)\big) \tag{9.5}$$

and from the hypotheses on $A(t) \equiv 1 - \Gamma(t)$ it follows that the map $I \ni t \mapsto H_{p+1}(t) \in \mathcal{K}_1(\mathfrak{h})$ is continuously differentiable in the norm of $\mathcal{K}_1(\mathfrak{h})$. Thus, the limit (9.4) exists, or equivalently the limit (9.3) also exists. Then, an easy computation using the geometric series leads to the expected result, *i.e.*, the limit in (9.4) is equal to the r.h.s. of (6.8).

Finally, for the last statement of the lemma, it is enough to observe from (9.5) that the map $I \ni t \mapsto H_p(t) \in \mathcal{K}_1(\mathfrak{h})$ is continuously differentiable in the norm of $\mathcal{K}_1(\mathfrak{h})$ if the map $I \ni t \mapsto \Gamma(t) - 1 \in \mathcal{K}_p(\mathfrak{h})$ is continuously differentiable in the norm of $\mathcal{K}_p(\mathfrak{h})$. Thus the entire proof holds already for p instead of $p + 1$. □

Proof of Lemma 6.12. Let us denote by $\mathbb{S}_0$ the open subset of $\mathbb{S}$ (with full measure) such that $\mathbb{S}_0 \ni t \mapsto \Gamma(t) \in \mathcal{K}(\mathfrak{h})$ is continuously differentiable. One first observes that for any $t \in \mathbb{S}_0$ and $q > p$ one has

$$\begin{aligned} M_q(t) &:= \operatorname{tr}\big[\big(1-\Gamma(t)\big)^q\Gamma(t)^*\Gamma'(t)\big] \\ &= \operatorname{tr}\Big[\big(1-\Gamma(t)\big)^{q-1}\Gamma(t)^*\Gamma'(t) - \Gamma(t)\big(1-\Gamma(t)\big)^{q-1}\Gamma(t)^*\Gamma'(t)\Big] \\ &= M_{q-1}(t) - \operatorname{tr}\big[\big(1-\Gamma(t)\big)^{q-1}\Gamma'(t)\big] \end{aligned}$$

where the unitarity of $\Gamma(t)$ has been used in the third equality. Thus the statement will be proved by reiteration if one shows that the map $\mathbb{S}_0 \ni t \mapsto \operatorname{tr}\big[\big(1-\Gamma(t)\big)^{q-1}\Gamma'(t)\big] \in \mathcal{K}(\mathfrak{h})$ is integrable, with

$$\int_{\mathbb{S}_0} \operatorname{tr}\big[\big(1-\Gamma(t)\big)^{q-1}\Gamma'(t)\big]\,\mathrm{d}t = 0. \tag{9.6}$$

For that purpose, let us set for simplicity $A(t) := 1 - \Gamma(t)$ and observe that for t, s in the same arc of $\mathbb{S}_0$ and with $s \neq t$ one has

$$\operatorname{tr}[A(s)^q] - \operatorname{tr}[A(t)^q] = \operatorname{tr}\big[A(s)^q - A(t)^q\big] = \operatorname{tr}\Big[P_{q-1}\big(A(s),A(t)\big)\,\big(A(s)-A(t)\big)\Big]$$

where $P_{q-1}\big(A(s),A(t)\big)$ is a polynomial of degree $q-1$ in the two non commutative variables $A(s)$ and $A(t)$. Note that we were able to use the cyclicity because of the assumptions $q-1 \geq p$ and $A(t) \in \mathcal{K}_p(\mathfrak{h})$ for all $t \in \mathbb{S}$. Now, let us observe that

$$\begin{aligned} &\left|\frac{1}{|s-t|}\operatorname{tr}\Big[P_{q-1}\big(A(s),A(t)\big)\,\big(A(s)-A(t)\big)\Big] - \operatorname{tr}\Big[P_{q-1}\big(A(t),A(t)\big)\,A'(t)\Big]\right| \\ &\quad\leq \left\|\frac{A(s)-A(t)}{|s-t|}\right\| \left|\operatorname{tr}\big[P_{q-1}\big(A(s),A(t)\big) - P_{q-1}\big(A(t),A(t)\big)\big]\right| \\ &\qquad + \left\|\frac{A(s)-A(t)}{|s-t|} - A'(t)\right\| \left|\operatorname{tr}\big[P_{q-1}\big(A(t),A(t)\big)\big]\right| . \end{aligned}$$

By assumptions, both terms vanish as $s \to t$. Furthermore, one observes that $P_{q-1}\big(A(t),A(t)\big) = qA(t)^{q-1}$. Collecting these expressions one has shown that

$$\lim_{s\to t} \frac{\operatorname{tr}[A(s)^q] - \operatorname{tr}[A(t)^q]}{|s-t|} - q\operatorname{tr}[A(t)^{q-1}A'(t)] = 0 ,$$

or in simpler terms $\frac{1}{q}\big(\operatorname{tr}[A(\cdot)^q]\big)'(t) = \operatorname{tr}[A(t)^{q-1}A'(t)]$. By inserting this equality into (9.6) and by taking the continuity of $\mathbb{S} \ni t \mapsto \Gamma(t)$ into account, one directly obtains that this integral is equal to 0, as expected. □

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Counting Function of Magnetic Eigenvalues for Non-definite Sign Perturbations

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Abstract. We consider the perturbed operator $H(b, V) := H(b, 0) + V$, where $H(b, 0)$ is the 3d Hamiltonian of Pauli with non-constant magnetic field, and V is *a non-definite sign electric potential* decaying exponentially with respect to the variable along the magnetic field. We prove that the only resonances of $H(b, V)$ near the low ground state zero of $H(b, 0)$ are its eigenvalues and are concentrated in the semi axis $(-\infty, 0)$. Further, we establish new asymptotic expansions, upper and lower bounds on their number near zero.

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1. Introduction

In this article, we consider a three-dimensional Pauli operator $H(b, V) = H(b, 0) + V$ acting in $L^2(\mathbb{R}^3) := L^2(\mathbb{R}^3, \mathbb{C}^2)$. It describes a quantum non-relativistic spin-$\frac{1}{2}$ particle, subject to an electric potential V and a non-constant magnetic field $\mathbf{B} : \mathbb{R}^3 \to \mathbb{R}^3$ of constant direction. With no loss of generality, we may assume that the magnetic field has the form

$$\mathbf{B}(x_1, x_2, x_3) = \big(0, 0, b(x_1, x_2)\big). \tag{1.1}$$

Throughout this paper, $b : \mathbb{R}^2 \to \mathbb{R}$ will be assumed to be an admissible magnetic field. That is, there exists a constant $b_0 > 0$ satisfying $b(x_1, x_2) = b_0 + \tilde{b}(x_1, x_2)$, where $\tilde{b}$ is a function such that the Poisson equation

$$\Delta\tilde{\varphi} = \tilde{b}, \quad \Delta := \partial_1^2 + \partial_2^2, \tag{1.2}$$

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admits a solution $\tilde{\varphi} \in C^2(\mathbb{R}^2)$ verifying $\sup_{(x_1,x_2)\in\mathbb{R}^2} |D^\alpha \tilde{\varphi}(x_1,x_2)| < \infty$, $\alpha \in \mathbb{N}^2$, $|\alpha| \leq 2$, (we refer for instance to [25, Section 2.1] for more details on admissible magnetic fields). Notice that $\tilde{b} = 0$ coincides with the constant magnetic field case.

Let $\mathbf{A} = (A_1, A_2, A_3) : \mathbb{R}^3 \to \mathbb{R}^3$ be a magnetic potential generating the magnetic field $\mathbf{B}$. That is,

$$\mathbf{B}(X) = \operatorname{curl} \mathbf{A}(X), \quad X = (X_\perp, x_3) \in \mathbb{R}^3, \quad X_\perp = (x_1, x_2) \in \mathbb{R}^2. \tag{1.3}$$

The self-adjoint unperturbed Pauli operator $H(b,0)$ is defined originally on $C_0^\infty(\mathbb{R}^3, \mathbb{C}^2)$ by

$$H(b,0) := \begin{pmatrix} (-i\nabla - \mathbf{A})^2 - b & 0 \\ 0 & (-i\nabla - \mathbf{A})^2 + b \end{pmatrix}, \tag{1.4}$$

and then closed in $L^2(\mathbb{R}^3)$. Since b is independent of x_3, then with no loss of generality, we may assume that A_j, $j = 1, 2$, are independent of x_3 and $A_3 = 0$. Set $\varphi_0(X_\perp) := b_0|X_\perp|^2/4$ and $\varphi := \varphi_0 + \tilde{\varphi}$, so that we have $\Delta\varphi = b$. Introduce the operators

$$a = a(b) := -2i\mathrm{e}^{-\varphi} \frac{\partial}{\partial \bar{z}} \mathrm{e}^{\varphi} \quad \text{and} \quad a^* = a^*(b) := -2i\mathrm{e}^{\varphi} \frac{\partial}{\partial z} \mathrm{e}^{-\varphi}, \tag{1.5}$$

originally defined on $C_0^\infty(\mathbb{R}^2, \mathbb{C})$, where $z := x_1 + ix_2$ and $\bar{z} := x_1 - ix_2$. Define the operators

$$H_1(b) := a^*a \quad \text{and} \quad H_2(b) := aa^*. \tag{1.6}$$

By choosing $A_1 = -\partial_2\varphi$ and $A_2 = \partial_1\varphi$, the operator $H(b,0)$ can be rewritten in $L^2(\mathbb{R}^3) = L^2(\mathbb{R}^2) \otimes L^2(\mathbb{R})$ as

$$H(b,0) = \begin{pmatrix} H_1(b) \otimes 1 + 1 \otimes \big(-\partial_3^2\big) & 0 \\ 0 & H_2(b) \otimes 1 + 1 \otimes \big(-\partial_3^2\big) \end{pmatrix} =: \begin{pmatrix} \mathcal{H}_1(b) & 0 \\ 0 & \mathcal{H}_2(b) \end{pmatrix}, \tag{1.7}$$

where $-\partial_3^2$ is originally defined on $C_0^\infty(\mathbb{R}, \mathbb{C})$. From [24, Proposition 1.1], we know that the spectra $\operatorname{sp}(H_j)$ of H_j, $j = 1, 2$, satisfy the following properties:

$$\begin{aligned} &\operatorname{sp}(H_1) \subseteq \{0\} \cup [\zeta, +\infty) \text{ with } 0 \text{ an eigenvalue of infinite multiplicity,} \\ &\operatorname{sp}(H_2) \subseteq [\zeta, +\infty), \end{aligned} \tag{1.8}$$

where

$$\zeta := 2b_0 \mathrm{e}^{-2\operatorname{osc}\tilde{\varphi}} > 0, \tag{1.9}$$

with $\operatorname{osc}\tilde{\varphi} := \sup_{X_\perp\in\mathbb{R}^2} \tilde{\varphi}(X_\perp) - \inf_{X_\perp\in\mathbb{R}^2} \tilde{\varphi}(X_\perp)$. Since the spectrum of the operator $-\partial_3^2$ coincides with $[0,+\infty)$ and is absolutely continuous, then (1.7) and (1.8) imply that this of $H(b,0)$ is equal to $[0,+\infty)$ and is absolutely continuous (see [25, Corollary 2.2]).

Remark. It is well known (see, e.g., [12]) in the constant magnetic field case, the spectrum of H_1 consists of the Landau levels $2b_0\mathbb{N}$. Further, the multiplicity of each eigenvalue $2b_0q$, $q \in \mathbb{N}$, is infinite. In particular, this implies that the spectrum of H_2 consists of the Landau levels $2b_0\mathbb{N}^*$. Further, $\zeta = 2b_0$.

On the domain of the operator $H(b,0)$, we introduce the perturbed operator

$$H(b,V) = H(b,0) + V, \tag{1.10}$$

where we identify V with the multiplication operator by the function V.

In [29], we investigated the resonances (see Definition 4.1 below) of the operator $H(b,V)$ near zero. We required $V \equiv \{V_{jk}\}_{1\leq j,k\leq 2}$ to be a hermitian matrix-valued electric potential satisfying

$$|V_{jk}(X)| \leq C\,\langle X_\perp\rangle^{-m_\perp} \mathrm{e}^{-2\delta\langle x_3\rangle}, \quad m_\perp > 0, \quad \delta > 0, \tag{1.11}$$

where $\langle u\rangle := \sqrt{1+|u|^2}$, $u \in \mathbb{R}^d$, $d \geq 1$. For V of definite sign, we obtained in [29, Theorem 2.2] an asymptotic expansion of the number of resonances near zero. Further, we showed that they are concentrated in some sector. For V of *non-definite sign*, we obtained in [29, Theorem 2.1] an upper bound of the number of resonances near zero without their localization.

The aim of this paper is to study the same problem by considering the class of anti-diagonal matrix-valued electric potentials

$$V(X) := \begin{pmatrix} 0 & \overline{U}(X) \\ U(X) & 0 \end{pmatrix}, \quad X \in \mathbb{R}^3, \quad U(X) \in \mathbb{C}, \tag{1.12}$$

where the function U satisfies the estimate

$$|U(X)| \leq C\,\langle X_\perp\rangle^{-m_\perp} \mathrm{e}^{-2\delta\langle x_3\rangle}, \quad m_\perp > 0, \quad \delta > 0, \tag{1.13}$$

with $C > 0$ a constant.

Remark. Notice that potentials V satisfying (1.12) are of *non-definite sign*. Indeed, its eigenvalues are $\pm|U(X)|$.

Novelty in this paper is that we prove the only resonances of $H(b,V)$ near zero are its eigenvalues. Further, they are localized in the semi axis $(-\infty,0)$. We give new estimates on the number of negative eigenvalues of $H(b,V)$ near zero. In particular, they show that the behaviour of magnetic eigenvalues for unsigned perturbations is different from that for signed perturbations. The crucial tool is that we exploit the form (1.12) of V in such a way we reduce the analysis of the resonances of $H(b,V)$ near $z = 0$ to that of the semi-effective Hamiltonian $\mathcal{H}_1 - \overline{U}\big(\mathcal{H}_2 - z\big)^{-1}U$ (see Section 4).

The paper is organized in the following manner. Our main results (Theorems 2.1 and 2.2) are stated in Section 2. In Section 3, we recall auxiliary results on Toeplitz operators and characteristic values of meromorphic operator-valued functions. In Section 4, we reduce the analysis of the resonances near zero to a characteristic value problem. Section 5 is devoted to the proofs of Theorems 2.1 and 2.2.

2. Statement of the main results

In order to formulate our main results, some notations are needed. For T a linear compact self-adjoint operator in a Hilbert space, we denote

$$n_+(s,T) := \operatorname{rank} \mathbb{P}_{(s,\infty)}(T), \quad s > 0, \tag{2.1}$$

where $\mathbb{P}_{(s,\infty)}(T)$ is the orthogonal projection of T in the interval (s,∞). The set of negative eigenvalues of the operator $H(b,V)$ is denoted $\mathrm{sp}_{\mathrm{disc}}\big(H(b,V)\big)$, namely its discrete spectrum. The orthogonal projection onto $\operatorname{Ker} H_1(b)$ defined by (1.6) is denoted $p := p(b)$. The corresponding orthogonal projection in the constant magnetic field case will be denoted $p_0 := p(b_0)$.

For a bounded operator $\mathscr{B} \in \mathscr{L}\big(L^2(\mathbb{R}^3)\big)$, we define on $L^2(\mathbb{R}^2)$ the operator $W(\mathscr{B})$ by

$$\big(W(\mathscr{B})f\big)(X_\perp) := \frac{1}{2}\int_{\mathbb{R}} \overline{U}(X_\perp, x_3)\mathscr{B}(Uf)(X_\perp, x_3)dx_3, \quad X_\perp \in \mathbb{R}^2. \tag{2.2}$$

Clearly, if I denotes the identity on $L^2(\mathbb{R}^3)$, then $W(I)$ is the multiplication operator by the function

$$X_\perp \longmapsto \frac{1}{2}\int_{\mathbb{R}} |U|^2(X_\perp, x_3)dx_3. \tag{2.3}$$

The function (2.3) will be denoted $W(I)$ again. Let $\mathcal{H}_2$ be the operator defined by (1.7). If U satisfies (1.13), then [25, Lemma 2.4] implies that the positive self-adjoint operators $pW(I)p$ and $pW\big(\mathcal{H}_2^{-1}\big)p$ are compact on $L^2(\mathbb{R}^2)$.

We are thus led to our first main result, where the resonances are defined in Definition 4.1 below.

Theorem 2.1. *Assume that* (1.12) *and* (1.13) *hold for V and U respectively. Then, there exists a discrete set $\mathcal{E} \subset \mathbb{R}^*$ such that for any $\nu \in \mathbb{R}^* \setminus \mathcal{E}$, the operator $H(b,\nu V)$ has the following properties:*

(i) *Localization: near zero, the resonances are its negative eigenvalues.*

(ii) *Asymptotic: suppose that $n_+\Big(r, pW\big(\mathcal{H}_2^{-1}\big)p\Big) \to +\infty$, $r \searrow 0$. Then, there exists a sequence $(r_\ell)_\ell$ tending to 0 such that*

$$\#\mathrm{sp}_{\mathrm{disc}}\big(H(b,\nu V)\big) \cap \big(-\infty, -r_\ell^2\big) = n_+\Big(r_\ell, pW\big(\mathcal{H}_2^{-1}\big)p\Big)\big(1+o(1)\big), \quad \ell \longrightarrow \infty. \tag{2.4}$$

(iii) *Upper-bound: let I be the identity on $L^2(\mathbb{R}^3)$. If $W(I) \le U_\perp$ with $U_\perp$ satisfying the assumptions of Lemma* 3.1*, then*

$$\#\mathrm{sp}_{\mathrm{disc}}\big(H(b,\nu V)\big) \cap \big(-\infty, -r^2\big) \le n_+\left(r, \frac{1}{\zeta}pW(I)p\right)\big(1+o(1)\big), \quad r \searrow 0. \tag{2.5}$$

Remarks. Notice that in virtue of Lemma 3.1, the right-hand side of (2.5) implies that the number of negative eigenvalues of $H(b,\nu V)$ near zero is of order $\mathcal{O}\big(r^{-1/m_\perp}\big)$, $r \searrow 0$. This order is better than the order $\mathcal{O}\big(r^{-2/m_\perp}\big)$ obtained in [29] for general perturbations V satisfying (1.11). Otherwise, if the function $U_\perp$ is

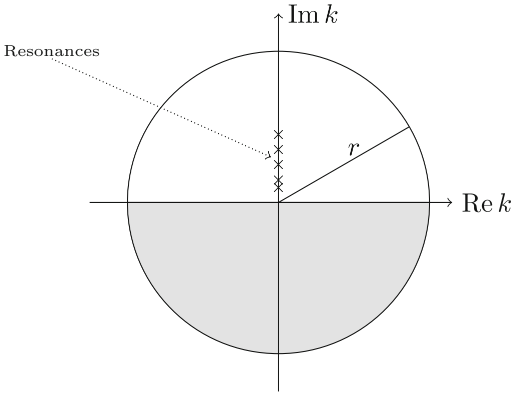

FIGURE 1. **Resonances near 0 with respect to the variable k:** For $r \ll 1$, the only resonances $z(k) = k^2$ of $H(b, 0) + V$ near zero are its negative eigenvalues and they satisfy $k \in i]0, +\infty)$.

compactly supported, then (2.5) and [25, Lemma 3.4] imply that the number of negative eigenvalues of $H(b, \nu V)$ near zero is of order $\mathcal{O}\big((\ln|\ln r|)^{-1}|\ln r|\big)$, $r \searrow 0$, which is similar to that from [29].

In the constant magnetic field case $\mathbf{B} = (0, 0, b_0)$, we obtain, in additional, a lower bound of the number of negative eigenvalues near zero.

Before stating our result, some additional notations are needed. If the function U satisfies $U(X_\perp, x_3) = U_\perp(X_\perp)\mathcal{U}(x_3)$, where $U_\perp$ and $\mathcal{U}$ are not necessarily real functions, we define

$$K_1 := \frac{\Big\langle \big(-\partial_3^2 + 2b_0\big)^{-1}\mathcal{U}, \mathcal{U}\Big\rangle}{2}, \tag{2.6}$$

and

$$n_*\left(\left(\frac{r}{K_1}\right)^{\frac{1}{2}}, p_0 U_\perp p_0\right) := n_+\left(\frac{r}{K_1}, \big(p_0 U_\perp p_0\big)^* p_0 U_\perp p_0\right). \tag{2.7}$$

Theorem 2.2 (Lower bound). *Let the magnetic field* $\mathbf{B}$ *be constant. Assume that* (1.12) *and* (1.13) *hold for* V *and* U *respectively. Then, there exists a discrete set* $\mathcal{E} \subset \mathbb{R}^*$ *such that for any* $\nu \in \mathbb{R}^* \setminus \mathcal{E}$*, the following holds:*

Suppose that $U(X_\perp, x_3) = U_\perp(X_\perp)\mathcal{U}(x_3)$*. If we have*

$$n_*\left(\left(\frac{r}{K_1}\right)^{\frac{1}{2}}, p_0 U_\perp p_0\right) = \phi(r)\big(1 + o(1)\big), \quad r \searrow 0,$$

where the function $\phi(r)$ *is as in Lemma* 3.5*, then*

$$\#\mathrm{sp}_{\mathrm{disc}}\big(H(b,\nu V)\big) \cap \big(-\infty,-r^2\big) \geq n_* \left(\left(\frac{r}{K_1}\right)^{\frac{1}{2}}, p_0 U_\perp p_0\right) \big(1+o(1)\big), \quad r \searrow 0. \tag{2.8}$$

In particular, if $U_\perp \geq 0$ *and satisfies the assumptions of Lemma* 3.1*, then*

$$\#\mathrm{sp}_{\mathrm{disc}}\big(H(b,\nu V)\big) \cap \big(-\infty,-r^2\big) \geq n_+ \left(\left(\frac{r}{K_1}\right)^{\frac{1}{2}}, p_0 U_\perp p_0\right) \big(1+o(1)\big), \quad r \searrow 0. \tag{2.9}$$

Remarks. Notice that estimates (2.9) and (2.5) imply, in the constant magnetic field case, the number of negative eigenvalues of $\big(H(b,\nu V)\big)$ near 0 is such that

$$\begin{aligned} &C_{m_\perp} K_1^{1/m_\perp} r^{-1/m_\perp}\big(1+o(1)\big) \\ &\quad \leq \#\mathrm{sp}_{\mathrm{disc}}\big(H(b,\nu V)\big) \cap \big(-\infty,-r^2\big) \\ &\quad \leq C_{m_\perp} K_2^{1/m_\perp} r^{-1/m_\perp}\big(1+o(1)\big), \quad r \searrow 0, \end{aligned} \tag{2.10}$$

where $C_{m_\perp}$ is the constant defined in Lemma 3.1, and

$$K_2 := (4b_0)^{-1} \int_{\mathbb{R}} |\mathcal{U}(x_3)|^2 dx_3. \tag{2.11}$$

It is easy to check that $K_1 < K_2$. On the other hand, the lower bound in (2.10) implies that the negative eigenvalues of $H(b,\nu V)$ accumulate to zero. One can compare (2.10) with the results of [25] on the asymptotic of the counting function of the eigenvalues of $H(b,V)$ near zero, when $V \equiv \{V_{jk}\}_{1\leq j,k\leq 2}$ has a fixed sign. Indeed, in [25, Corollary 3.6], the author shows that if the coefficients of the potential $V \geq 0$ satisfy

$$|V_{jk}(X)| = \mathcal{O}\big(\langle X\rangle^{-\nu}\big), \quad 1 \leq j,k \leq 2,$$

for some $\nu > 3$, then the behaviour near zero of the counting function of the negative eigenvalues of $H(b,V)$ is of order

$$\mathcal{O}\big(r^{-2/(\nu-1)}\big)\big(1+o(1)\big), \quad r \searrow 0.$$

In particular, this shows that the behaviour of eigenvalues for unsigned perturbations is different from that for signed perturbations.

3. Auxiliary results

3.1. Some results on Berezin–Toeplitz operators by Raikov [25], [22]

Consider $U_\perp \in L^\infty(\mathbb{R}^2)$. The asymptotic eigenvalues of the Berezin–Toeplitz operator pUp is the subject of the next lemma. An integrated density of states (IDS) for the operator $H_1 = H_1(b)$ is defined as follows. For $X_\perp \in \mathbb{R}^2$, let $\chi_{T,X_\perp}$ be the characteristic function of the square $X_\perp + \big(-\frac{T}{2},\frac{T}{2}\big)^2$ with $T > 0$. Denote $\mathbb{P}_I(H_1)$

the spectral projection of H_1 in the interval $I \subset \mathbb{R}$. A non-increasing function $g : \mathbb{R} \longrightarrow [0, \infty)$ is called an IDS for H_1 if it satisfies for any $X_\perp \in \mathbb{R}^2$

$$g(t) = \lim_{T\to\infty} T^{-2}\,\mathrm{Tr}\left[\chi_{T,X_\perp}\mathbb{P}_{(-\infty,t)}(H_1)\chi_{T,X_\perp}\right],$$

for each point t of continuity of g (see, e.g., [25]). If the magnetic field is constant, then there exists naturally an IDS for the operator H_1 given by

$$g(t) = \frac{b_0}{2\pi}\sum_{q=0}^{\infty}\chi_{\mathbb{R}_+}(t - 2b_0 q), \quad t \in \mathbb{R},$$

where $\chi_{\mathbb{R}_+}$ is the characteristic function of $\mathbb{R}_+$.

Lemma 3.1 ([22, Theorem 2.6]). *Consider $U_\perp \in C^1(\mathbb{R}^2)$ such that*

$$0 \le U_\perp(X_\perp) \le C_1\langle X_\perp\rangle^{-\alpha}, \;\; |\nabla U_\perp(X_\perp)| \le C_1\langle X_\perp\rangle^{-\alpha-1}, \;\; X_\perp \in \mathbb{R}^2,$$

where $\alpha > 0$ and $C_1 > 0$. Assume that

- *$U_\perp(X_\perp) = u_0(X_\perp/|X_\perp|)|X_\perp|^{-\alpha}\big(1 + o(1)\big)$ as $|X_\perp| \to \infty$, where u_0 is a continuous function on $\mathbb{S}^1$ which does not vanish identically,*
- *b is an admissible magnetic field,*
- *there exists an IDS g for the operator $H_1(b)$.*

Then we have

$$n_+(s, pU_\perp p) = C_\alpha s^{-2/\alpha}\big(1 + o(1)\big), \;\; s \searrow 0,$$

where

$$C_\alpha := \frac{b_0}{4\pi}\int_{\mathbb{S}^1} u_0(t)^{2/\alpha}dt. \tag{3.1}$$

3.2. Results on characteristic values by Bony–Bruneau–Raikov [7]

Let $\mathscr{H}$ be a separable Hilbert space. We denote $S_\infty(\mathscr{H})$ (resp. $GL(\mathscr{H})$) the set of compact (resp. invertible) linear operators acting in $\mathscr{H}$.

Let $D \subseteq \mathbb{C}$ be a connected open set, $Z \subset D$ be a discrete and closed subset, $A : \overline{D}\backslash Z \longrightarrow GL(\mathscr{H})$ be a finite meromorphic operator-valued function (see, e.g., [7, Definition 2.1]) and Fredholm at each point of Z. The index of A, with respect to a positive oriented contour γ, is defined by

$$\mathrm{Ind}_\gamma\, A := \frac{1}{2i\pi}\mathrm{Tr}\int_\gamma A'(z)A(z)^{-1}dz = \frac{1}{2i\pi}\mathrm{Tr}\int_\gamma A(z)^{-1}A'(z)dz. \tag{3.2}$$

Here, the operator A does not vanish on the integration contour γ. Let $\mathcal{D}$ be a domain of $\mathbb{C}$ containing 0. Consider a holomorphic operator-valued function $T : \mathcal{D} \longrightarrow S_\infty(\mathscr{H})$. For a domain $\Omega \subset \mathcal{D} \setminus \{0\}$, a complex number $z \in \Omega$ is said to be a *characteristic value* of $z \mapsto \mathscr{T}(z) := I - \frac{T(z)}{z}$ if the operator $\mathscr{T}(z)$ is not invertible. The multiplicity of a characteristic value z_0 is defined by

$$\mathrm{mult}(z_0) := \mathrm{Ind}_\gamma\big(I - \mathscr{T}(\cdot)\big), \tag{3.3}$$

where γ is a small contour positively oriented, containing z_0 as the unique point z satisfying $\mathscr{T}(z)$ is not invertible.

Define

$$\mathcal{Z}(\Omega) := \left\{ z \in \Omega : I - \frac{T(z)}{z} \text{ is not invertible} \right\}.$$

If there exists $z_0 \in \Omega$ such that $I - \frac{T(z_0)}{z_0}$ is not invertible, then $\mathcal{Z}(\Omega)$ is a discrete set (see, e.g., [15, Proposition 4.1.4]). So we define

$$\mathcal{N}(\Omega) := \#\mathcal{Z}(\Omega).$$

Assume that $T(0)$ is self-adjoint. Introduce $\Omega \Subset \mathbb{C} \setminus \{0\}$ and the sector

$$\mathcal{C}_\alpha(a,b) := \{x + iy \in \mathbb{C} : a \le x \le b, -\alpha x \le y \le \alpha x\}, \tag{3.4}$$

with $a > 0$ tending to 0 and $b > 0$. Let

$$n(\Lambda) := \operatorname{Tr} \mathbf{1}_\Lambda(T(0))$$

be the number of eigenvalues of the operator $T(0)$ lying in the interval $\Lambda \subset \mathbb{R}^*$, and counted with their multiplicity. Denote Π_0 the orthogonal projection onto $\operatorname{Ker} T(0)$.

Lemma 3.2 ([7, Corollary 3.4]). *Let T be as above and $I - T'(0)\Pi_0$ be invertible. Assume that $\Omega \Subset \mathbb{C} \setminus \{0\}$ is a bounded domain with smooth boundary $\partial\Omega$ which is transverse to the real axis at each point of $\partial\Omega \cap \mathbb{R}$.*

(i) *If $\Omega \cap \mathbb{R} = \emptyset$, then $\mathcal{N}(s\Omega) = 0$ for s small enough. This implies that the characteristic values $z \in \mathcal{Z}(\mathcal{D})$ near 0 satisfy $|\operatorname{Im} z| = o(|z|)$.*

(ii) *Moreover, if the operator $T(0)$ has a definite sign ($\pm T(0) \ge 0$), then the characteristic values z near 0 satisfy $\pm \operatorname{Re} z \ge 0$, respectively.*

(iii) *If $T(0)$ is of finite rank, then there are no characteristic values in a pointed neighbourhood of 0. Moreover, if the operator $T(0)\mathbf{1}_{[0,+\infty)}(\pm T(0))$ is of finite rank, then there are no characteristic values in a neighbourhood of 0 intersected with $\{\pm \operatorname{Re} z > 0\}$, respectively.*

Lemma 3.3 ([7, Theorem 3.7]). *Let T be as above and $I - T'(0)\Pi_0$ be invertible. For $\alpha > 0$ fixed, let $\mathcal{C}_\alpha(r,1) \subset \mathcal{D}$ be defined as in (3.4). Then, for all $\delta > 0$ small enough, there exists $s(\delta) > 0$ such that, for all $0 < s < s(\delta)$, we have*

$$\begin{aligned}\mathcal{N}\big(\mathcal{C}_\alpha(r,1)\big) &= n\big([r,1]\big)\big(1 + \mathcal{O}\big(\delta|\ln\delta|^2\big)\big) \\ &\quad + \mathcal{O}\big(|\ln\delta|^2\big)n\big([r(1-\delta), r(1+\delta)]\big) + \mathcal{O}_\delta(1),\end{aligned} \tag{3.5}$$

where the $\mathcal{O}$'s are uniform with respect to s, δ but the $\mathcal{O}_\delta$ may depend on δ.

Lemma 3.4 ([7, Corollary 3.9]). *Let the assumptions of Lemma 3.3 hold true. Assume that there exists $\gamma > 0$ such that*

$$n([r,1]) = O(r^{-\gamma}), \quad r \searrow 0,$$

and that $n([r,1])$ grows unboundedly as $r \searrow 0$. Then there exists a positive sequence $(r_k)_k$ tending to 0 such that

$$\mathcal{N}(\mathcal{C}_\alpha(r_k,1)) = n([r_k,1])(1 + o(1)), \quad k \to \infty. \tag{3.6}$$

Lemma 3.5 ([7, Corollary 3.11]). *Let the assumptions of Lemma* 3.3 *hold true. Suppose that*

$$n\big([r,1]\big) = \Phi(r)\big(1+o(1)\big), \quad r \searrow 0,$$

with $\Phi(r) = r^{-\gamma}$, *or* $\Phi(r) = |\ln r|^{\gamma}$, *or* $\Phi(r) = \big(\ln|\ln r|\big)^{-1}|\ln r|$, *for some* $\gamma > 0$. *Then*

$$\mathcal{N}\big(\mathcal{C}_\alpha(r,1)\big) = \Phi(r)\big(1+o(1)\big), \quad r \searrow 0. \tag{3.7}$$

4. Resonances

From here to the end, we assume that V and U satisfy (1.12) and (1.13) respectively.

4.1. A preliminary property

We establish the main property allowing to reduce the study of the resonances of $H(b,V)$ near $z=0$ to that of the semi-effective Hamiltonian $\mathcal{H}_1 - \overline{U}\big(\mathcal{H}_2 - z\big)^{-1}U$.

Let $z \in \mathbb{C}$ be small enough. We have

$$\begin{aligned} \big(H(b,V)-z\big) & \begin{pmatrix} 1 & 0 \\ -(\mathcal{H}_2 - z)^{-1}U & (\mathcal{H}_2 - z)^{-1} \end{pmatrix} \\ & = \begin{pmatrix} \mathcal{H}_1 - z - \overline{U}(\mathcal{H}_2 - z)^{-1}U & \overline{U}(\mathcal{H}_2 - z)^{-1} \\ 0 & 1 \end{pmatrix}. \end{aligned} \tag{4.1}$$

Therefore,

$$H(b,V) - z \text{ is invertible} \Leftrightarrow \mathcal{H}_1 - z - \overline{U}(\mathcal{H}_2 - z)^{-1}U \text{ is invertible.} \tag{4.2}$$

Further,

$$\begin{aligned} \big(H(b,V)-z\big)^{-1} &= \begin{pmatrix} 1 & 0 \\ -(\mathcal{H}_2 - z)^{-1}U & (\mathcal{H}_2 - z)^{-1} \end{pmatrix} \\ \times & \begin{pmatrix} \big(\mathcal{H}_1 - z - \overline{U}(\mathcal{H}_2 - z)^{-1}U\big)^{-1} & -\big(\mathcal{H}_1 - z - \overline{U}(\mathcal{H}_2 - z)^{-1}U\big)^{-1}\overline{U}(\mathcal{H}_2 - z)^{-1} \\ 0 & 1 \end{pmatrix}. \end{aligned} \tag{4.3}$$

Hence, for z small enough, property (4.2) allows to reduce the non-invertibility of the operator $H(b,V) - z$ to that of $\mathcal{H}_1 - z - \overline{U}(\mathcal{H}_2 - z)^{-1}U$.

4.2. Reduction to a semi-effective problem

Consider z lying in the upper half-plane $\mathbb{C}^+$. Make the change of variables

$$z := z(k) = k^2 \;\text{ for }\; k \in \mathbb{C}^+_{1/2} := \big\{k \in \mathbb{C}^+ : k^2 \in \mathbb{C}^+\big\}. \tag{4.4}$$

Introduce the punctured disk

$$D(0,\epsilon)^* := \big\{k \in \mathbb{C} : 0 < |k| < \epsilon\big\}, \quad \epsilon < \min\Big(\delta, \sqrt{\zeta}\Big), \tag{4.5}$$

where the constants δ and ζ are respectively defined by (1.13) and (1.9).

Proposition 4.1 ([29, Proposition 4.1]). *Let $R(z)$ denote the resolvent of the operator $H(b,V)$. Then, the operator-valued function*

$$k \longmapsto \Big(R\big(z(k)\big) : \mathrm{e}^{-\delta\langle x_3\rangle} L^2(\mathbb{R}^3) \longrightarrow \mathrm{e}^{\delta\langle x_3\rangle} L^2(\mathbb{R}^3) \Big),$$

admits a meromorphic extension from $\mathbb{C}^+_{1/2} \cap D(0,\epsilon)^*$ to $D(0,\epsilon)^*$. We shall denote this extension $R(z)$ again.

Definition 4.1. We define the resonances of $H(b,V)$ near zero as the poles of the meromorphic extension $R(z)$.

Set $\mathscr{R}(z) := \big(\mathcal{H}_1 - z - \overline{U}(\mathcal{H}_2 - z)^{-1} U\big)^{-1}$ and $R_2(z) := (\mathcal{H}_2 - z)^{-1}$. From (4.3) we deduce that

$$\begin{aligned} &\mathrm{e}^{-\delta\langle x_3\rangle} R(z) \mathrm{e}^{-\delta\langle x_3\rangle} \\ &= \begin{pmatrix} \mathrm{e}^{-\delta\langle x_3\rangle} \mathscr{R}(z) \mathrm{e}^{-\delta\langle x_3\rangle} & -\mathrm{e}^{-\delta\langle x_3\rangle} \mathscr{R}(z) \overline{U} R_2(z) \mathrm{e}^{-\delta\langle x_3\rangle} \\ -\mathrm{e}^{-\delta\langle x_3\rangle} R_2(z) U \mathscr{R}(z) \mathrm{e}^{-\delta\langle x_3\rangle} & \begin{matrix} \mathrm{e}^{-\delta\langle x_3\rangle} R_2(z) U \mathscr{R}(z) \overline{U} R_2(z) \mathrm{e}^{-\delta\langle x_3\rangle} \\ + \mathrm{e}^{-\delta\langle x_3\rangle} R_2(z) \mathrm{e}^{-\delta\langle x_3\rangle} \end{matrix} \end{pmatrix}. \end{aligned} \tag{4.6}$$

This together with Proposition 4.1 and assumption (1.13) show that the poles of $R(z)$ coincide with those of $\mathscr{R}(z)$. Then, near $z = 0$, the investigation of the resonances of $H(b,V)$ is reduced to that of the semi-effective Hamiltonian $\mathcal{H}_1 - \overline{U}(\mathcal{H}_2 - z)^{-1} U$.

4.3. Study of the semi-effective problem

With the help of the decomposition

$$(\mathcal{H}_2 - z)^{-1} = \mathcal{H}_2^{-1} \Big(1 - z\mathcal{H}_2^{-1}\Big)^{-1} = \mathcal{H}_2^{-1} \sum_{k\geq 0} z^k \mathcal{H}_2^{-k}, \tag{4.7}$$

z being sufficiently small, we obtain

$$(\mathcal{H}_2 - z)^{-1} = \mathcal{H}_2^{-1/2} \Big(\mathcal{H}_2^{-1/2} + \mathcal{H}_2^{-1/2} M(z) \Big), \tag{4.8}$$

where

$$M(z) := z \sum_{k\geq 0} z^k \mathcal{H}_2^{-k-1}. \tag{4.9}$$

So, (4.8) implies that

$$\overline{U}(\mathcal{H}_2 - z)^{-1} U = \overline{U} \mathcal{H}_2^{-1/2} \Big(\mathcal{H}_2^{-1/2} U + \mathcal{H}_2^{-1/2} M(z) U \Big). \tag{4.10}$$

Now define the operator

$$\mathbf{w} := \mathcal{H}_2^{-1/2} U. \tag{4.11}$$

Thus, putting together (4.10) and (4.11) we obtain

$$\overline{U}(\mathcal{H}_2 - z)^{-1} U = \mathbf{w}^* \big(1 + M(z)\big) \mathbf{w}. \tag{4.12}$$

We therefore have proved the following

Lemma 4.1. *For z small enough, the operator $\overline{U}(H_2 - z)^{-1}U$ admits the representation*

$$\overline{U}(\mathcal{H}_2 - z)^{-1}U = \mathbf{w}^* \big(1 + M(z)\big)\mathbf{w}. \tag{4.13}$$

Further, the operator-valued function $z \longmapsto M(z)$ is analytic near $z = 0$.

Let $R_1(z)$ denote the resolvent of the operator $\mathcal{H}_1$. Under the notations of Lemma 4.1, the following lemma holds:

Lemma 4.2. *For z small enough, the operator-valued function*

$$D(0, \epsilon)^* \ni k \longmapsto \mathcal{T}_V\big(z(k)\big) := \Big(1 + M\big(z(k)\big)\Big)\mathbf{w}R_1\big(z(k)\big)\mathbf{w}^*,$$

is analytic with values in $S_\infty\big(L^2(\mathbb{R}^3)\big)$.

Proof. The analyticity of $\mathcal{T}_V\big(z(k)\big)$ holds since $M\big(z(k)\big)$ and $UR_1\big(z(k)\big)\overline{U}$ are well defined and analytic for $k \in D(0, \epsilon)^*$.

The compactness of $\mathcal{T}_V\big(z(k)\big)$ follows from that of $UR_1\big(z(k)\big)\overline{U}$, using the diamagnetic inequality and [32, Theorem 2.13]. □

We have the following characterization of the resonances.

Proposition 4.2. *For k near zero, the following assertions are equivalent:*

(i) *$z(k) = k^2$ is a resonance of $H(b, V)$,*
(ii) *1 is an eigenvalue of $\mathcal{T}_V\big(z(k)\big)$.*

Proof. The equivalence follows directly from the identity

$$\Big(I - \big(1 + M(z)\big)\mathbf{w}R_1(z)\mathbf{w}^*\Big)\Big(I + \big(1 + M(z)\big)\mathbf{w}\mathscr{R}(z)\mathbf{w}^*\Big) = I, \tag{4.14}$$

and the fact that the poles of $R(z)$ coincide with those of $\mathscr{R}(z)$. □

So, the multiplicity of a resonance $z := z(k)$ is defined by

$$\operatorname{mult}(z) := \operatorname{Ind}_\gamma \Big(I - \mathcal{T}_V\big(z(\cdot)\big)\Big), \tag{4.15}$$

where γ is a small positively oriented contour containing k as the unique point satisfying $z(k)$ is a resonance of $H(b, V)$ $\big($see (3.2)$\big)$.

Using the terminology of characteristic value recalled in Subsection 3.2, Proposition 4.2 can be formulated as follows:

Proposition 4.3. *For k near zero, the following assertions are equivalent:*

(i) *$z = z(k)$ is a resonance of $H(b, V)$,*
(ii) *k is a characteristic value of $I - \mathcal{T}_V\big(z(\cdot)\big)$.*

Further, according to (4.15), the multiplicity of the resonance $z(k)$ coincides with this of the characteristic value k.

5. Proof of the main results

First, let us introduce some tools. For $p = p(b)$, set $q := I - p$. Define on $L^2(\mathbb{R}^3)$ the projections $P := p \otimes 1$ and $Q := q \otimes 1$. If z lies in the resolvent set the operator $\mathcal{H}_1$, we have

$$\begin{aligned}(\mathcal{H}_1 - z)^{-1} &= (\mathcal{H}_1 - z)^{-1}P + (\mathcal{H}_1 - z)^{-1}Q \\ &= p \otimes \mathcal{R}(z) + (\mathcal{H}_1 - z)^{-1}Q,\end{aligned} \tag{5.1}$$

where the resolvent $\mathcal{R}(z) := \big(-\partial_3^2 - z\big)^{-1}$ admits the integral kernel

$$\mathcal{N}_z(x_3 - x_3') = i\mathrm{e}^{i\sqrt{z}|x_3 - x_3'|}/(2\sqrt{z}), \quad \operatorname{Im}\sqrt{z} > 0. \tag{5.2}$$

5.1. Proof of Theorem 2.1

5.1.1. Preliminary results. Firstly, we need to split the operator $\mathcal{T}_V\big(z(k)\big)$ of Lemma 4.2 with the help of (5.1). We get

$$\begin{aligned}\mathcal{T}_V\big(z(k)\big) &= \mathbf{w}p \otimes \mathcal{R}(k^2)\mathbf{w}^* + M\big(z(k)\big)\mathbf{w}p \otimes \mathcal{R}(k^2)\mathbf{w}^* \\ &\quad + \Big(1 + M\big(z(k)\big)\Big)\mathbf{w}R_1\big(z(k)\big)Q\mathbf{w}^*.\end{aligned} \tag{5.3}$$

The operators $M\big(z(k)\big)$ and $R_1\big(z(k)\big)Q$ are analytic near zero. Then, it is not difficult to see that the third term of the right-hand side of (5.3) is holomorphic near zero, with values in $S_\infty\big(L^2(\mathbb{R}^3)\big)$. By (5.2), the integral kernel of $N(k) := \mathrm{e}^{-\delta\langle x_3\rangle}\mathcal{R}(k^2)\mathrm{e}^{-\delta\langle x_3\rangle}$ is given by

$$\mathrm{e}^{-\delta\langle x_3\rangle}\frac{i\mathrm{e}^{ik|x_3 - x_3'|}}{2k}\mathrm{e}^{-\delta\langle x_3'\rangle}. \tag{5.4}$$

This together with (4.9) imply that the second term of the right-hand side of (5.3) is analytic in a vicinity of zero, with values in $S_\infty\big(L^2(\mathbb{R}^3)\big)$.

Now let us focus on the first term $\mathbf{w}p \otimes \mathcal{R}(k^2)\mathbf{w}^*$. According to (5.4), we can write

$$N(k) = \frac{1}{k}a + b(k), \tag{5.5}$$

where $a : L^2(\mathbb{R}) \longrightarrow L^2(\mathbb{R})$ is the rank-one operator defined by

$$a(u) := \frac{i}{2}\langle u, \mathrm{e}^{-\delta\langle\cdot\rangle}\rangle\mathrm{e}^{-\delta\langle x_3\rangle}, \tag{5.6}$$

and $b(k)$ is the Hilbert–Schmidt operator $\big($for $k \in D(0,\epsilon)^*\big)$ with integral kernel

$$\mathrm{e}^{-\delta\langle x_3\rangle}i\frac{\mathrm{e}^{ik|x_3 - x_3'|} - 1}{2k}\mathrm{e}^{-\delta\langle x_3'\rangle}. \tag{5.7}$$

Thus,

$$\mathbf{w}p \otimes \mathcal{R}(k^2)\mathbf{w}^* = \frac{i}{k} \times \frac{1}{2}\mathbf{w}\big(p \otimes \tau\big)\mathbf{w}^* + \mathbf{w}\big(p \otimes s(k)\big)\mathbf{w}^*, \tag{5.8}$$

where τ and $s(k)$ are operators acting from $\mathrm{e}^{-\delta\langle x_3\rangle}L^2(\mathbb{R})$ to $\mathrm{e}^{\delta\langle x_3\rangle}L^2(\mathbb{R})$, with integral kernels respectively given by 1 and

$$\frac{1-\mathrm{e}^{ik|x_3-x_3'|}}{2ik}. \tag{5.9}$$

We therefore have proved the following

Proposition 5.1. *Let $k \in D(0,\epsilon)^*$. Then,*

$$\mathcal{T}_V\big(z(k)\big) = i\frac{\mathbf{w}(p\otimes\tau)\mathbf{w}^*}{2k} + B(k), \tag{5.10}$$

where

$$\begin{aligned} B(k) := \mathbf{w}\big(p\otimes s(k)\big)\mathbf{w}^* + M\big(z(k)\big)\mathbf{w}p\otimes\mathcal{R}(k^2)\mathbf{w}^* \\ + \Big(1+M\big(z(k)\big)\Big)\mathbf{w}R_1\big(z(k)\big)Q\mathbf{w}^*, \end{aligned} \tag{5.11}$$

is holomorphic in $D(0,\epsilon) := D(0,\epsilon)^*\cup\{0\}$, with values in $S_\infty\big(L^2(\mathbb{R}^3)\big)$.

Notice that $\mathbf{w}(p\otimes\tau)\mathbf{w}^*$ is a positive self-adjoint compact operator. Indeed, if we define $e_\pm$ as the multiplication operators by the functions $e_\pm : x_3 \longmapsto \mathrm{e}^{\pm\delta\langle x_3\rangle}$, it is easy to check that

$$\mathbf{w}(p\otimes\tau)\mathbf{w}^* = \mathbf{w}e_+(p\otimes c^*c)e_+\mathbf{w}^* = \big((p\otimes c)e_+\mathbf{w}^*\big)^*\big((p\otimes c)e_+\mathbf{w}^*\big). \tag{5.12}$$

Here, $c : L^2(\mathbb{R}) \longrightarrow \mathbb{C}$ is defined by $c(f) := \langle f, e_-\rangle$, so that $c^* : \mathbb{C} \longrightarrow L^2(\mathbb{R})$ is given by $c^*(\lambda) = \lambda e_-$. Now, with the help of (5.12), we deduce that

$$n_+\left(r, \frac{\mathbf{w}(p\otimes\tau)\mathbf{w}^*}{2}\right) = n_+\left(r, \frac{(p\otimes c)e_+\mathbf{w}^*\mathbf{w}e_+(p\otimes c^*)}{2}\right), \quad r>0, \tag{5.13}$$

where the quantity $n_+(r,\cdot)$ is defined by (2.1). By the definition (4.11) of $\mathbf{w}$, we have $\mathbf{w}^*\mathbf{w} = \overline{U}\mathcal{H}_2^{-1}U$. This together with $\mathrm{sp}(\mathcal{H}_2) \subseteq [\zeta,+\infty)$ imply that

$$\frac{(p\otimes c)e_+\mathbf{w}^*\mathbf{w}e_+(p\otimes c^*)}{2} = pW\big(\mathcal{H}_2^{-1}\big)p \le \frac{pW(I)p}{\zeta}, \tag{5.14}$$

where for $\mathscr{B} \in \mathscr{L}\big(L^2(\mathbb{R}^3)\big)$, $W(\mathscr{B})$ is the operator defined by (2.2). Then, by combining (5.13) with (5.14) we obtain

$$\begin{aligned} n_+\left(r, \frac{\mathbf{w}(p\otimes\tau)\mathbf{w}^*}{2}\right) &= n_+\Big(r, pW\big(\mathcal{H}_2^{-1}\big)p\Big) \\ &\le n_+\left(r, \frac{pW(I)p}{\zeta}\right), \quad r>0. \end{aligned} \tag{5.15}$$

Otherwise, according to Proposition 4.3, the study of the resonances $z(k) = k^2$ of $H(b,\nu V)$ near zero, is reduced to that of the characteristic values of the operator

$$I - \mathcal{T}_{\nu V}\big(z(k)\big) = I + \nu^2\frac{T(ik)}{ik}.$$

Here, taking into account Proposition 5.1, $T(ik) := \frac{\mathbf{w}(p\otimes\tau)\mathbf{w}^*}{2} - ikB(k)$ so that $T(0) = \frac{\mathbf{w}(p\otimes\tau)\mathbf{w}^*}{2}$. Let Π_0 be the orthogonal projection onto $\operatorname{Ker} T(0)$. Since

$T'(0)\Pi_0$ is compact, then, there exists a sequence $(\nu_n)_n$ such that $I - \nu T'(0)\Pi_0$ is invertible for any $\nu \in \mathbb{R}\backslash\{\nu_n, n \in \mathbb{N}\}$. Note that we can take $\nu_n = \lambda_n^{-1}$, where $\{\lambda_n, n \in \mathbb{N}\}$ is the set of eigenvalues of the operator $T'(0)\Pi_0$.

5.1.2. Back to the proof of Theorem 2.1. Notations are those from Subsection 3.2.

(i) It follows immediately from Lemma 3.2 with $z = -ik/\nu^2$.

(ii) Theorem 2.1 (i) shows, in particular, for $|k|$ small enough the resonances $z(k) = k^2$ are concentrated in the sector $\{k \in D(0,\epsilon)^* : -ik/\nu^2 \in \mathcal{C}_\alpha(r, r_0)\}$, for any $\alpha > 0$. Hence, if $\mathrm{Res}\big(H(b,\nu V)\big)$ denotes the set of resonances of $H(b,\nu V)$, we have

$$\begin{aligned}
\#\big\{z(k) = k^2 \in \mathrm{Res}\big(H(b,\nu V)\big) : r < |k| \le r_0\big\} \\
&= \#\big\{z(k) = k^2 \in \mathrm{Res}\big(H(b,\nu V)\big) : -ik/\nu^2 \in \mathcal{C}_\alpha(r, r_0)\big\} + \mathcal{O}(1) \\
&= \mathcal{N}\big(\mathcal{C}_\alpha(r,r_0)\big) + \mathcal{O}(1), \quad r \searrow 0.
\end{aligned} \tag{5.16}$$

On the other hand, we have

$$n\big([r,r_0]\big) = \mathrm{Tr}\, \mathbf{1}_{[r,r_0]}\big(T(0)\big) = n_+\left(r, \frac{\mathbf{w}(p\otimes\tau)\mathbf{w}^*}{2}\right) + \mathcal{O}(1). \tag{5.17}$$

This together with the inequality in (5.15) imply that

$$n\big([r,r_0]\big) \le n_+\left(r, \frac{pW(I)p}{\zeta}\right) + \mathcal{O}(1).$$

Then, Theorem 2.1 (ii) follows from (5.16) together with Lemma 3.4, (5.17) and the equality in (5.15).

(iii) If we have $W(I) \le U_\perp$, with $U_\perp$ satisfying the assumptions of Lemma 3.1, then

$$n_+\left(r, \frac{pW(I)p}{\zeta}\right) = C_{m_\perp}(\zeta r)^{-1/m_\perp}\big(1 + o(1)\big), \quad r \searrow 0, \tag{5.18}$$

where $m_\perp$ is the constant defined by (1.13). Similarly to the inequality in (5.15), we can show that

$$n\big([r,r_0]\big) \le \mathrm{Tr}\, \mathbf{1}_{[r,r_0]}\left(\frac{pW(I)p}{\zeta}\right) =: \tilde{n}\big([r,r_0]\big). \tag{5.19}$$

Note that due to (5.18),

$$\tilde{n}\big([r,r_0]\big) = C_{m_\perp}(\zeta r)^{-1/m_\perp}\big(1 + o(1)\big), \quad r \searrow 0. \tag{5.20}$$

Now if $\phi(r) = r^{-\gamma}$, $\gamma > 0$, then $\phi\big(r(1\pm\nu)\big) = r^{-\gamma}(1\pm\nu)^{-\gamma} = \phi(r)\big(1 + \mathcal{O}(\nu)\big)$. If $\tilde{n}\big([r,1]\big) = \phi(r)\big(1 + o(1)\big)$ with $\phi\big(r(1\pm\delta)\big) = \phi(r)\big(1 + o(1) + \mathcal{O}(\delta)\big)$, then

$$\tilde{n}\big(\big[r(1-\nu), r(1+\nu)\big]\big) = \tilde{n}\big([r,1]\big)\big(o(1) + \mathcal{O}(\nu)\big). \tag{5.21}$$

Then, Theorem 2.1 (iii) follows from (5.16) together with Lemma 3.3, (5.19), (5.20) and (5.21).

5.2. Proof of Theorem 2.2

To obtain (2.8), it suffices to prove that if the function U satisfies $U(X_\perp, x_3) = U_\perp(X_\perp)\mathcal{U}(x_3)$, then the following operator inequality holds:

$$K_1\big(p_0U_\perp p_0\big)^*\big(p_0U_\perp p_0\big) \le p_0 W\big(\mathcal{H}_2^{-1}\big)p_0. \tag{5.22}$$

Indeed, if (5.22) is true, then with respect to the constant magnetic field, the quantity $n\big([r,r_0]\big) = \operatorname{Tr}\mathbf{1}_{[r,r_0]}\left(\frac{\mathbf{w}(p_0\otimes\tau)\mathbf{w}^*}{2}\right) = \operatorname{Tr}\mathbf{1}_{[r,r_0]}\Big(p_0W\big(\mathcal{H}_2^{-1}\big)p_0\Big)$ satisfies

$$n_*\big([r,r_0]\big) := \operatorname{Tr}\mathbf{1}_{[r,r_0]}\Big[K_1\big(p_0U_\perp p_0\big)^*\big(p_0U_\perp p_0\big)\Big] \le n\big([r,r_0]\big). \tag{5.23}$$

Further, if we have

$$\begin{aligned} n_*\left(\left(\frac{r}{K_1}\right)^{\frac12}, p_0U_\perp p_0\right) &:= n_+\left(\frac{r}{K_1}, \big(p_0U_\perp p_0\big)^* p_0U_\perp p_0\right) \\ &= \phi(r)\big(1+o(1)\big), \quad r\searrow 0, \end{aligned}$$

where the function $\phi(r)$ is as in Lemma 3.5, then

$$n_*\big([r,r_0]\big) = \phi(r)\big(1+o(1)\big), \quad r\searrow 0. \tag{5.24}$$

Thus, (2.8) follows by arguing as in the proof of Theorem 2.1 (iii) above.

Now let us proof (5.22). If the magnetic field is constant, then $\mathcal{H}_2$ satisfies

$$\mathcal{H}_2^{-1} \ge \mathcal{H}_2^{-1}p_0 = p_0 \otimes \big(-\partial_3^2 + 2b_0\big)^{-1}.$$

This together with the definition (2.2) of $W\big(\mathcal{H}_2^{-1}\big)$ imply that, if $U(X_\perp, x_3) = U_\perp(X_\perp)\mathcal{U}(x_3)$, then for any $f\in L^2\big(\mathbb{R}^2\big)$

$$\Big\langle W\big(\mathcal{H}_2^{-1}\big)f, f\Big\rangle \ge K_1\big\langle \overline{U_\perp}p_0U_\perp f, f\big\rangle. \tag{5.25}$$

This means that we have the operator inequality

$$W\big(\mathcal{H}_2^{-1}\big) \ge K_1\overline{U_\perp}p_0U_\perp.$$

Thus,

$$p_0W\big(\mathcal{H}_2^{-1}\big)p_0 \ge K_1\big(p_0U_\perp p_0\big)^*\big(p_0U_\perp p_0\big),$$

which is exactly (5.22). This concludes the proof of Theorem 2.2.

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Harmonic Analysis and Random Schrödinger Operators

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Abstract. This survey is based on a series of lectures given during the *School on Random Schrödinger Operators* and the *International Conference on Spectral Theory and Mathematical Physics* at the Pontificia Universidad Catolica de Chile, held in Santiago in November 2014. As the title suggests, the presented material has two foci: Harmonic analysis, more precisely, unique continuation properties of several natural function classes and Schrödinger operators, more precisely properties of their eigenvalues, eigenfunctions and solutions of associated differential equations. It mixes topics from (rather) pure to (rather) applied mathematics, as well as classical questions and results dating back a whole century to very recent and even unpublished ones. The selection of material covered is based on the selection made for the minicourse, and is certainly a personal choice corresponding to the research interests of the authors.

Emphasis is laid not so much on proofs, but rather on concepts, questions, results, examples and applications. In several cases, however, we do supply proofs of special cases or sketches of proofs, and use them to illustrate the underlying concepts. As the minicourse *Harmonic Analysis and Random Schrödinger Operators* itself, we designed the text to be accessible to advanced graduate students who have already acquired some experience with partial differential equations. On the other hand, even experts in the field will find new results, mostly toward the end of the text.

The line of thought starts with discussing unique continuation properties of holomorphic and harmonic functions. Already here we illustrate different notions of unique continuation. Hereafter, elliptic partial differential equations are introduced and unique continuation properties of their solutions are discussed. Then we shift our attention to domains and differential equations with an inherent multiscale structure. The question here is, whether appropriately collected local data of a function give good estimates to global properties of the function. In the framework of harmonic analysis the Whittaker–Nyquist–Kotelnikov–Shannon Sampling and the Logvinenko–Sereda Theorem are examples of such results. From here it is natural to pursue the question whether similar and related results can be expected for (classes of) solutions of differential equations. This leads us to quantitative unique countinuation bounds which are obtained by the use of Carleman estimates. In the context of random Schrödinger operators they have risen to some prominence recently since they facilitated the resolution of some long-standing problems in the field. We present several unique continuation theorems tailored for this applications. Finally, after several results on the spectral properties of random Schrödinger operators, an application to control of the heat equation is given.

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Contents

1. Introduction

1.1. Unique continuation

Intuitively, a unique continuation property describes the phenomenon that certain global properties of appropriately chosen function classes are uniquely determined by knowledge of the function locally, that is on arbitrarily small balls around a reference point. The following definition is classic. We denote by $B(x,r) = \{y \in \mathbb{R}^d \mid |x-y| < r\}$ the open ball with center $x \in \mathbb{R}^d$ and radius $r > 0$. If $x = 0$ we write $B(r)$ instead of $B(0,r)$.

Definition 1.1. Let $\Omega \subset \mathbb{R}^d$ be open. A class of functions $\mathcal{F} = \mathcal{F}(\Omega) \subset \{f \colon \Omega \to \mathbb{C} \mid f \text{ measurable}\}$ satisfies:

- *a (weak) unique continuation property*, if every $f \in \mathcal{F}$ that vanishes on a non-empty and open subset $W \subset \Omega$ vanishes everywhere. In other words, we have the implication

$$\exists\, W \subset \Omega \text{ non-empty and open, with } f \equiv 0 \text{ on } W \Rightarrow f \equiv 0; \tag{1}$$

- *a strong unique continuation property*, if every $f \in \mathcal{F}$ that vanishes on every polynomial order at some point $x_0 \in \Omega$ vanishes everywhere. In other words, we have the implication

$$\exists\, x_0 \in \Omega \text{ such that } \forall\, N \in \mathbb{N} : \lim_{\varepsilon \to 0} \varepsilon^{-N} \int_{B(x_0,\varepsilon)} |f| \mathrm{d}x = 0 \Rightarrow f \equiv 0. \tag{2}$$

In the present manuscript we also introduce the following notions which have been considered previously in the literature and/or are suitable for the discussion which follows.

Remark 1.2. Let $\Omega \subset \mathbb{R}^d$ be open. A class of functions $\mathcal{F} \subset \{f \colon \Omega \to \mathbb{C} \mid f \text{ measurable}\}$ satisfies:

- *a semi-strong unique continuation property*, if every $f \in \mathcal{F}$ that vanishes on some exponential order at some point $x_0 \in \Omega$ vanishes everywhere. In other words, we have the implication

$$\exists\, x_0 \in \Omega \text{ and } a, b > 0 \text{ with } \lim_{\varepsilon \to 0} \mathrm{e}^{a\varepsilon^{-b}} \int_{B(x_0,\varepsilon)} |f| \mathrm{d}x = 0 \Rightarrow f \equiv 0; \tag{3}$$

- *a very strong unique continuation property of order* $N_0 > 0$, if there is an ε-polynomial lower bound of order N_0 for the $\mathcal{L}^1$-norm of $0 \not\equiv f \in \mathcal{F}$ on ε-balls. More precisely, if for each $x_0 \in \Omega$ and $0 \not\equiv f \in \mathcal{F}$ there is a constant $C = C(x_0, f)$ and a radius $\varepsilon_0 = \varepsilon_0(x_0, f) \in (0, \infty)$ such that

$$C\varepsilon^{N_0} \leq \int_{B(x_0,\varepsilon)} |f| \mathrm{d}x \quad \text{ for all } \varepsilon \in (0, \varepsilon_0). \tag{4}$$

The notion "weak" to "very strong" makes sense since (4) ⇒ (2) ⇒ (3) ⇒ (1). In fact, the only non-trivial implication is (4) ⇒ (2), so let us give a short proof.

Proof of (4) ⇒ (2). Assume that f satisfies the very strong unique continuation property of order $N_0 \in \mathbb{N}$ and that there is $x_0 \in \Omega$ such that for all $N \in \mathbb{N}$ (hence in particular for some $N > N_0$) we have $\lim_{\varepsilon \to 0} \varepsilon^{-N} \int_{B(x_0,\varepsilon)} |f| \mathrm{d}x = 0$. Using $f \not\equiv 0$, we find by the very strong unique continuation property

$$\lim_{\varepsilon \to 0} \varepsilon^{-N} \int_{B(x_0,\varepsilon)} |f| \mathrm{d}x \geq \lim_{\varepsilon \to 0} C\varepsilon^{N_0 - N} = \infty$$

since $N > N_0$, a contradiction. □

It makes sense to consider uniform variants of these properties, for instance uniform w.r.t. the center of the ball x_0 or uniform w.r.t. the functions in the set $\mathcal{F}$. Sometimes such uniformity is easy to achieve, sometimes not. A nice example, where compactness and periodicity are used to enhance a simple unique continuation property to a unique continuation property, uniform over several scales, is given in Section 4 of [CHK03].

In particular one has the following uniform variants of the *very strong unique continuation property of order* N_0: We say that a class of functions $\mathcal{F} \subset \{f \colon \Omega \to \mathbb{C} \mid f \text{ measurable}\}$ satisfies the

- very strong unique continuation property of order N_0, *uniform in the base point*, if for every $0 \not\equiv f \in \mathcal{F}$ there is a constant $C = C(f)$ and a radius $\varepsilon_0 = \varepsilon_0(f) \in (0, \infty)$ such that

$$C\varepsilon^{N_0} \leq \int_{B(x_0,\varepsilon)} |f| \mathrm{d}x \quad \text{for all } x_0 \in \Omega \text{ and } \varepsilon \in (0, \varepsilon_0).$$

It may well happen that the behaviour of functions in $\mathcal{F}$ near the boundary of Ω is less regular than, say, the r-interior $\Omega_r := \{x \in \Omega \mid \operatorname{dist}(x, \partial\Omega) > r\}$ for some $r > 0$. In this case we would not have the above type of uniformity. We also say that $\mathcal{F}$ satisfies the

- very strong unique continuation property of order N_0, *uniform in the set* $\mathcal{F}$, if for every $x_0 \in \Omega$ there is a radius $\varepsilon_0 = \varepsilon_0(x_0) \in (0, \infty)$ such that for all $0 \not\equiv f \in \mathcal{F}$ there is a constant $C = C(x_0, f) \in (0, \infty)$ with

$$C\varepsilon^{N_0} \leq \int_{B(x_0,\varepsilon)} |f| \mathrm{d}x \quad \text{for all } \varepsilon \in (0, \varepsilon_0)$$

- and a very strong unique continuation property of order N_0, *uniform in the base point and in the set* $\mathcal{F}$, if there is a radius $\varepsilon_0 \in (0, \infty)$ such that for every $0 \not\equiv f \in \mathcal{F}$ there is a constant $C = C(f) \in (0, \infty)$ with

$$C\varepsilon^{N_0} \leq \int_{B(x_0,\varepsilon)} |f| \mathrm{d}x \quad \text{for all } x_0 \in \Omega \text{ and } \varepsilon \in (0, \varepsilon_0). \tag{5}$$

One might wonder whether the constant $C = C(f)$ could be chosen uniform in $\mathcal{F}$, as well. This cannot be expected if $\mathcal{F}$ is closed under scalar multiplication, as it is the case for vector spaces, since then for sufficiently small $\lambda > 0$,

$$\int_{B(x_0,\varepsilon)} |\lambda f| \mathrm{d}x = \lambda \int_{B(x_0,\varepsilon)} |f| \mathrm{d}x < C\varepsilon^{N_0}.$$

Thus we see that it will be natural to complement the requirement $f \in \mathcal{F}$ with some kind of normalization, e.g., $\int |f|^p = 1$. Alternatively, the normalization can be already taken care of in the function class $\mathcal{F}$. Then we would be dealing, e.g., with the unit sphere in a normed linear space. In this situation one can obviously drop the condition $f \not\equiv 0$ which appeared several times above.

Remark 1.3. Another way to allow $\mathcal{F}$ to be a vector space would be to multiply the left-hand side of (5) with the norm of f. Later, in Section 3, we will do this, but in an $\mathcal{L}^2$-setting. This means that we will study inequalities of the form

$$C\varepsilon^{N_0} \int_{\Omega} |f|^2 \mathrm{d}x \leq \int_{B(x_0,\varepsilon)} |f|^2 \mathrm{d}x \quad \text{for all } x_0 \in \Omega \text{ and } \varepsilon \in (0, \varepsilon_0) \tag{6}$$

and similar expressions where $B(x_0, \varepsilon)$ has been replaced by a more general set, e.g., a disjoint union of ε-balls. We will call estimates as in (6) quantitative unique continuation estimates.

1.2. Harmonic and holomorphic functions

Example 1.4 (Polynomials of degree one on $\mathbb{R}$). Let $\mathcal{F} = \mathcal{P}_1(\mathbb{R})$ be the space of affine polynomials on $\mathbb{R}$ with degree at most one, that is $\Delta f = 0$, where Δ denotes the Laplace operator or the second derivative. Every $f \in \mathcal{P}_1(\mathbb{R})$ can be written as $f(x) = ax + b$ where $a, b \in \mathbb{R}$. Now there are three possibilities:

- If $a \neq 0$, there is exactly one root and f vanishes on no ball $B(x_0, \varepsilon)$.
- If $a = 0$, $b \neq 0$, then f never vanishes.
- If $a = 0$, $b = 0$, then $f \equiv 0$ on $\mathbb{R}^d$.

Thus, $\mathcal{F}$ satisfies the weak unique continuation property as well as the semi-strong and the strong unique continuation property. Moreover, $\mathcal{F}$ satisfies the very strong unique continuation property of order 2, since a non-zero function $f \in \mathcal{P}_1(\mathbb{R})$ can vanish at most of order 1.

Example 1.5 (Harmonic and holomorphic functions). One can generalize this to higher dimensions and an open connected $\Omega \subset \mathbb{R}^d$. The space of harmonic functions on Ω is $\{f \in C^2(\Omega) \mid \Delta f \equiv 0\}$. It is known, see for example [Rud70], that such functions are real analytic and thus the space of harmonic functions satisfies the weak, the semi-strong and the strong unique continuation property. The same holds for holomorphic functions $\mathbb{C} \to \mathbb{C}$.

By definition, the various unique continuation properties above concern local behaviour of a function at a point. Considering certain natural classes of functions one observes that there is a connection to global properties, for instance the growth behaviour at infinity.

Example 1.6 (A counterexample). For $k \in \mathbb{N}$ let $f_k : \mathbb{C} \to \mathbb{C}$, $z \mapsto z^k$. Since f_k is holomorphic, it is analytic and hence satisfies the weak, the semi-strong and the strong unique continuation property. For large k, however, f_k vanishes arbitrarily fast at $z_0 = 0$. Thus, for any N_0 the space $\{f : \mathbb{C} \to \mathbb{C} \mid f \text{ holomorphic}\}$ fails to satisfy the very strong unique continuation property (4) of order N_0. Furthermore, all f_k are uniformly bounded on $B(1)$ by 1. Thus, a local bound is not sufficient for very strong unique continuation. However, we observe that for large k, f_k grows fast at infinity.

One might hope that nonzero holomorphic functions cannot vanish faster at 0 than they grow at infinity. This observation is made more precise in the following theorem and its corollary. It is known as Hadamard's three circle theorem and can for instance be found in [Lit12], where it is stated as an already known result.

Theorem 1.7 (Hadamard's three circle theorem). *Let $r_1 < r_2 < r_3$, f be a holomorphic function on the annulus $r_1 \leq |z| \leq r_3$ and $M_f(r_i) := \max_{|z|=r_i} |f(z)|$. Then*

$$\log\left(\frac{r_3}{r_1}\right) \log M_f(r_2) \leq \log\left(\frac{r_3}{r_2}\right) \log M_f(r_1) + \log\left(\frac{r_2}{r_1}\right) \log M_f(r_3). \qquad (7)$$

If we choose $\varepsilon = r_3/r_2 = r_2/r_1$, then (7) becomes

$$2 \log M_f(r_2) \leq \log M_f(\varepsilon r_2) + \log M_f(r_2/\varepsilon).$$

Thus the theorem is a statement about convexity of the map $\log(r) \mapsto \log M_f(r)$.

Corollary 1.8. *Let $f : \mathbb{C} \to \mathbb{C}$ be holomorphic. Assume that f grows slower at ∞ than it vanishes at 0, i.e., we have*

$$\liminf_{\varepsilon \to 0} M_f(\varepsilon) \cdot M_f(1/\varepsilon) = 0.$$

Then $f \equiv 0$.

Proof. Let $z_0 \in \mathbb{C}$ with $|z_0| = 1$. We apply Hadamard's three circle theorem with $r_1 = \varepsilon$, $r_2 = 1$ and $r_3 = 1/\varepsilon$ and obtain for all $\varepsilon > 0$

$$2 \log M_f(1) \leq \log M_f(\varepsilon) + \log M_f(1/\varepsilon)$$

and thus

$$|f(z_0)|^2 \leq M_f(1)^2 \leq M_f(\varepsilon) \cdot M_f(1/\varepsilon).$$

Letting ε tend to 0, we find by our assumption that $f \equiv 0$ on $\{z \in \mathbb{C} \mid |z| = 1\}$. Since f is holomorphic, $f \equiv 0$ on $\{z \in \mathbb{C} \mid |z| \leq 1\}$ by the maximum principle. By analyticity we obtain $f \equiv 0$. □

Instead of holomorphic functions $f_k : \mathbb{C} \to \mathbb{C}, z \mapsto z^k$, we could also have considered the harmonic functions $F_k : \mathbb{R}^2 \to \mathbb{R}^2, (x, y) \mapsto \mathrm{Re}(x + iy)^k$ where we use the identification $\mathbb{C} \cong \mathbb{R}^2$. Since there is a natural connection between holomorphic and harmonic functions, namely the real and imaginary part of every holomorphic function are harmonic, we would have found similar relations between vanishing at 0 and growth at ∞ for harmonic functions on $\mathbb{R}^2$.

Another example concerns the spherical harmonics on the sphere, cf. [dV85].

Example 1.9 (Spherical harmonics). Let $\mathbb{S}^2 := \{x \in \mathbb{R}^3 \mid |x| = 1\}$ be the 2-sphere. There is a special orthonormal base of $\mathcal{L}^2(\mathbb{S}^2)$, called the spherical harmonics $\{Y_{l,m} \mid l \in \mathbb{N}, -l \leq m \leq l\}$ such that

$$\begin{cases} -\Delta Y_{l,m} &= l(l+1) Y_{l,m} \quad \text{and} \\ \frac{\partial}{\partial \phi} Y_{l,m} &= im Y_{l,m}, \end{cases}$$

where $\partial/\partial\phi$ denotes the derivative with respect to the ϕ coordinate in spherical coordinates.

We study the sequence $Y_{l,l}$, $l \in \mathbb{N}$. In spherical coordinates they are of the form

$$Y_{l,l} = c_l \cos(\theta)^l \exp(\mathrm{i} l\phi), \quad \theta \in [-\pi/2, \pi/2], \quad \phi \in [0, 2\pi),$$

where $c_l > 0$ is a normalization factor.

Letting E_r be a tubular neighborhood around the equator, that is $E_r := \{(\sigma, \theta) \in \mathbb{S}^2 \mid |\theta| < r\}$, then the mass of $Y_{l,l}$ concentrates exponentially around the equator if l tends to ∞, i.e., there is $C = C(r) > 0$ such that

$$\lim_{l\to\infty} \mathrm{e}^{C(r)l} \int_{\mathbb{S}^2 \setminus E_r} Y_{l,l} = 0. \tag{8}$$

The interesting points to consider are at the poles and we will consider the order of vanishing of the eigenfunctions at these points.

If we consider the class of functions $\mathcal{F} = \{Y_{l,l} \mid l \in \{1, \ldots, l_{\max}\}\}$ for some $l_{\max} \in \mathbb{N}$, then the uniform very strong unique continuation principle as in (5) is satisfied, as the following calculation shows.

Since the only zero of $Y_{l,l}$ is at the pole, we have for all $l = 1, \ldots, l_{\max}$, all $x_0 \in \mathbb{S}^2$ and all $\varepsilon < \pi/2$,

$$\int_{B(x_0,\varepsilon)} |Y_{l,l}| \mathrm{d}x \geq \int_{B(p,\varepsilon)} |Y_{l,l}| \mathrm{d}A,$$

where p is a pole (by symmetry, we can assume that p is the north pole). Note that balls on the sphere are defined with respect to the geodesic distance. Now,

$$\begin{aligned}
\int_{B(p,\varepsilon)} |Y_{l,l}| \mathrm{d}x &= \int_0^{2\pi} \mathrm{d}\phi \int_{\pi/2-\varepsilon}^{\pi/2} \mathrm{d}\theta c_l \cos(\theta)^l \sin(\theta) \\
&= 2\pi c_l \int_{\pi/2-\varepsilon}^{\pi/2} \cos(\theta)^l \sin(\theta) \\
&= \frac{2\pi c_l}{l+1} \cos(\pi/2 - \varepsilon)^{l+1} = \frac{2\pi c_l}{l+1} \sin(\varepsilon)^{l+1}.
\end{aligned}$$

The function $\varepsilon \mapsto \sin(\varepsilon)^{l+1}$ vanishes of order $l+1$ at 0. Thus for every $Y_{l,l}$, there is an $l+1$-polynomial lower bound, uniform on $\mathbb{S}^2$, i.e., there is $C = C(Y_{l,l}) > 0$ such that

$$\int_{B(x_0,\varepsilon)} |f| \geq C(f)\varepsilon^{l+1} \text{ for all } x_0 \in \mathbb{S}^2,\ \varepsilon < \pi/2.$$

Since in this case, $\mathcal{F}$ is a finite set, we can choose $C = \min_{l=1}^{l_{\max}} C(Y_{l,l})$ and find the uniform very strong unique continuation principle of order $N_0 = l+1$ as in (5).

On the other hand the set $\{Y_{l,l} \mid l \in \mathbb{N}\}$ does not satisfy the uniform very strong unique continuation principle. In fact, given $N_0 > 0$, we see by the above calculation that for $l_0 = \lceil N_0 \rceil \in \mathbb{N}$, the function Y_{l_0,l_0} vanishes of order $l_0 + 1 > N_0$ at the poles, thus (5) cannot hold.

The limit in (8) tells us that for high energies (high eigenvalues) the eigenfunctions are more and more unevenly distributed on the sphere. Of course, the choice of eigenbasis for the Laplace operator on the sphere and the 'diagonal' subsequence plays a crucial role here. Since the eigenvalues of the Laplacian on the sphere are highly degenerate one has a lot of freedom when choosing an orthonormal basis of eigenfunctions. With an appropriate choice of basis and enumeration, it may be well possible that eigenfunctions for high eigenvalues do obey an equidistribution or quantum ergodicity property on the sphere, excluding a behaviour like (8). In fact, this has been established to hold almost surely for a random choice of eigenbasis by Zelditch.

Note that the lth eigenvalue level of $-\Delta$ on $\mathbb{S}^2$ is $(2l-1)$-fold degenerate. Thus, the set of all possible choices of orthonormal bases of $\mathcal{L}^2(\mathbb{S}^2)$, consisting of eigenfunctions of Δ, can be identified with the product $U(1) \times U(3) \times U(5) \times \cdots$ where $U(n)$ denotes the unitary group on $\mathbb{C}^n$. This product naturally carries the structure of a probability measure, the Haar measure μ_{Haar}, see [Zel92] for details. The following result can be found in [Zel92]. We formulate a simplified version for multiplication operators.

Theorem 1.10 (Almost sure quantum ergodicity on the sphere). *Let $f \in C^\infty(\mathbb{S}^2)$. For μ_{Haar}-almost every orthonormal basis $(\phi_j)_{j\in\mathbb{N}}$ of $-\Delta$-eigenfunctions on $\mathcal{L}^2(\mathbb{S})$, that is $-\Delta\phi_j = E_j\phi_j$, we have*

$$\lim_{E\to\infty} \frac{1}{N(E)} \sum_{j\in\mathbb{N}; E_j\leq E} |\langle \phi_j, f\phi_j\rangle - \bar{f}|^2 = 0$$

where $\bar{f} = \mathrm{Vol}(\mathbb{S}^2)^{-1} \int_{\mathbb{S}^2} f(x)\mathrm{d}x$ and $N(E)$ is the number of eigenvalues not exceeding the energy E.

It is much harder to find a specific, deterministic eigenbasis for the Laplacian on the sphere with the quantum ergodicity property. A corresponding conjecture and first steps of its proof can be found in [BSSP03]. Using a different method a deterministic eigenbasis with the quantum ergodicity property was found very recently in [BML15].

These examples for the behaviour of Laplace eigenfunctions on the sphere were remarkable because they clarified that one has to be careful with analogies between ergodicity or integrability properties of a classical system and its quantum analogue.

2. Vanishing speed for solutions of elliptic PDE

One can generalize the study of unique continuation properties to solutions of a large class of partial differential operators. A milestone result is [Car39]. There unique continuation properties for solutions of a system of first-order differential equations with sufficiently regular coefficients on open subsets Ω of $\mathbb{R}^2$ are proven. Note that second-order partial differential equations can be transformed into a system of first-order differential equations, see for instance [Had03], page 348. For this purpose, Carleman introduced a new method which is nowadays called Carleman estimates. While Carleman's original result applies to the two-dimensional case only, it has been generalized to arbitrary dimensions in [Mül54] and by now there are plenty of results concerning Carleman estimates and their applications.

An example of a Carleman estimate, see [KRS86, Ken86] and the references therein, is the following: for all $u \in C_0^\infty(\mathbb{R}^d)$ and p, p' with $1/p - 1/p' = 2/d$, and all sufficiently large $\lambda > 0$ we have

$$\|\mathrm{e}^{-\lambda x_d} u\|_{\mathcal{L}^{p'}(\mathbb{R}^d)} \leq C \|e^{-\lambda x_d} \Delta u\|_{\mathcal{L}^p(\mathbb{R}^d)}, \tag{9}$$

where x_d denotes the dth coordinate of x. In fact, Ineq. (9) can be extended to $\{u \in \mathcal{L}^{p'}(\mathbb{R}^d) \mid \Delta u \in \mathcal{L}^p(\mathbb{R}^d) \text{ and } \exists \mu \in \mathbb{R}: \ \operatorname{supp} u \subset \{x_d > \mu\}\}$.

Example 2.1 (How to conclude UCP from Carleman). We follow [Ken86] and show how the Carleman estimate (9) can be used to obtain a unique continuation property. Let $V \in \mathcal{L}^{d/2}(\mathbb{R}^d)$ and, as before, $1/p - 1/p' = 2/d$. Our goal is to show that if $u \in C_0^\infty(\mathbb{R}^d)$ satisfies $|\Delta u| \leq |Vu|$ and $\operatorname{supp} u \subset \{x_d > 0\}$, then $u \equiv 0$.

Proof. In a first step, we show that u vanishes on a strip $S_\rho = \{x \in \mathbb{R}^d \mid x_d \in [0, \rho]\}$, $\rho > 0$. We choose $\rho > 0$ to be the largest number such that

$$C\|V\|_{\mathcal{L}^{d/2}(S_\rho + x_d \cdot e_d)} \leq \frac{1}{2} \text{ for all } x_d \in \mathbb{R}.$$

where C is the constant from the Carleman estimate (9) and e_d the unit vector in the dth dimension. Such a ρ exists since $V \in \mathcal{L}^{d/2}(\mathbb{R}^d)$. Now, inequality (9) gives for all $\lambda > 0$

$$\left\|\mathrm{e}^{-\lambda x_d} u\right\|_{\mathcal{L}^{p'}(S_\rho)} \leq C\left\|\mathrm{e}^{-\lambda x_d} V u\right\|_{\mathcal{L}^p(S_\rho)} + C\left\|\mathrm{e}^{-\lambda x_d} \Delta u\right\|_{\mathcal{L}^p(\mathbb{R}^d \setminus S_\rho)}.$$

By Hölder's inequality and our assumption on ρ we obtain

$$\left\|\mathrm{e}^{-\lambda x_d} u\right\|_{\mathcal{L}^{p'}(S_\rho)} \leq C\|V\|_{\mathcal{L}^{d/2}(S_\rho)} \left\|\mathrm{e}^{-\lambda x_d} u\right\|_{\mathcal{L}^{p'}(S_\rho)} + C\left\|\mathrm{e}^{-\lambda x_d} \Delta u\right\|_{\mathcal{L}^p(\mathbb{R}^d \setminus S_\rho)}.$$

Since $C\|V\|_{\mathcal{L}^{d/2}(S_\rho)} \leq 1/2$ we get

$$\left\|\mathrm{e}^{-\lambda x_d} u\right\|_{\mathcal{L}^{p'}(S_\rho)} \leq 2C\left\|\mathrm{e}^{-\lambda x_d} \Delta u\right\|_{\mathcal{L}^p(\mathbb{R}^d \setminus S_\rho)}.$$

We use $\mathrm{e}^{-\lambda x_d} \leq \mathrm{e}^{-\lambda \rho}$ for $x_d > \rho$ and obtain

$$\forall \lambda > 0: \quad \left\|\mathrm{e}^{-\lambda (x_d - \rho)} u\right\|_{\mathcal{L}^{p'}(S_\rho)} \leq 2C\left\|\Delta u\right\|_{\mathcal{L}^p(\mathbb{R}^d \setminus S_\rho)}.$$

Note that the right-hand side of the last inequality is independent of λ and that $x_d - \rho < 0$ on S_ρ. Hence, if $u \not\equiv 0$ on S_ρ, we get a contradiction by choosing λ large enough. By our choice of ρ, we can iterate this procedure and find that $u \equiv 0$ on $\mathbb{R}^d$. □

Remark 2.2 (Weight functions). The above example shows unique continuation on strips since the level sets of the weight function $\mathrm{e}^{-\lambda x_d}$ are strips. Hence, it might be tempting to search for radially symmetric weight functions in order to obtain unique continuation on annuli or balls. Indeed, such weight functions have been used in many situations, see the discussion in Remark 3.11 below. However, typically one wants the weight function to have nowhere vanishing gradient. For radially symmetric functions, this poses a problem at the origin, which can be resolved in various ways. One could exclude the origin from the domain and consider weight functions which are smooth except at the origin cf., e.g., Remark 3.11, or use a two-weight Carleman inequality, cf., e.g., [RT15].

Example 2.3 (Elliptic differential operators). Let H be the elliptic partial differential operator

$$Hf(x) := \sum_{j,j=1}^{d} \frac{\partial}{\partial x_i} \left(a_{ij}(x) \frac{\partial}{\partial x_j} f(x) \right) + V(x)f(x),$$

acting on $C^2(\Omega)$, where $\Omega \subset \mathbb{R}^d$ is open and connected, $V : \Omega \to \mathbb{R}$ is bounded and measurable, the functions $a_{ij} : \Omega \to \mathbb{R}$, $1 \leq i, j \leq d$, are Lipschitz continuous, $a_{ij} = a_{ji}$, and there is $\lambda > 0$ such that for all $x \in \Omega$ and all $\xi \in \mathbb{R}^d$

$$\frac{1}{\lambda}|\xi|^2 \leq \sum_{i,j=1}^{d} a_{ij}(x)\xi_i\xi_j \leq \lambda|\xi|^2.$$

By means of Carleman estimates it has been shown that the class $\{f \in C^2(\Omega) \mid Hf = 0\}$ satisfies the strong unique continuation property, see for instance [Wol93], where more general results are discussed. One can generalize this result to Sobolev spaces $W^{2,2}(\Omega)$ or $W^{2,p}(\Omega)$, $p > 1$.

Next we supply an example which shows that the two properties from Definition 1.1 are actually distinct.

Example 2.4 (Functions satisfying UCP, but not SUCP). Let $d \in \{3, 4\}$, $\Omega \subset \mathbb{R}^d$ be open, $a_{i,j} : \Omega \to \mathbb{R}$ Lipschitz for $i, j = 1, \ldots, d$, $A \in \mathcal{L}^{d/2}_{\mathrm{loc}}(\Omega)$ and $B \in \mathcal{L}^{d}_{\mathrm{loc}}(\Omega)$. Then solutions $u \in W^{2,2}_{\mathrm{loc}}(\Omega)$ of the differential inequality

$$\left| \sum_{i,j=1}^{d} a_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j} \right| \leq A|u| + B|\nabla u| \tag{10}$$

satisfy the unique continuation property, but not necessarily the strong unique continuation property, see [Wol93] and the references therein. Note that for $A, B \geq 0$, the set of solutions of the differential inequality (10) contains in particular solutions of the differential equation

$$\sum_{i,j=1}^{d} a_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j} = Au + B\nabla u.$$

For other examples of this type see [JK85, Ken86].

2.1. A result of Donnelly and Fefferman: Eigenfunctions of the Laplacian

We now consider a d-dimensional, connected, compact manifold M with a smooth (that is C^∞) Riemannian metric. The compactness will replace the condition of controlled growth at infinity of functions we have discussed in the context of Hadamard's three circle theorem. We want to study differentiable functions on M.

Example 2.5. A prominent example of such a manifold M is the d-dimensional torus $\mathbb{T}^d := \mathbb{R}^d/\mathbb{Z}^d$. Note that

$$C^k(\mathbb{T}^d) \cong C^k_{\mathrm{per}}(\mathbb{R}^d) = \left\{u \in C^k(\mathbb{R}^d) \mid u(x+k) = u(x) \text{ for all } x \in \mathbb{R}^d, k \in \mathbb{Z}^d\right\}.$$

In particular, we can learn about periodic problems in Euclidean space by studying this example.

The following theorem quantifies the vanishing speed of solutions of the differential equation $-\Delta u = Eu$, $E > 0$, where Δ denotes the Laplace–Beltrami operator on the manifold M. Here, the vanishing speed is quantified in $\mathcal{L}^\infty$-norm. It can be found in Proposition 4.1 of [DF88].

Theorem 2.6. *There are constants $C_1, C_2 \geq 0$, depending only on d, the diameter of M and the maximum over all sectional curvatures on M such that for every $E > 0$, every $u : M \to \mathbb{R}$, $0 \not\equiv u$ with $-\Delta u = Eu$ on M, and every $x_0 \in M$, u can vanish at most of order $C_1 + C_2\sqrt{E}$ with respect to the ∞-norm.*

More precisely, for every $u \not\equiv 0$ with $-\Delta u = Eu$ and every $x_0 \in M$ there is $\varepsilon_0 > 0$ such that for every $\varepsilon < \varepsilon_0$, we have

$$\varepsilon^{C_1 + C_2\sqrt{E}} \leq \max_{x \in B(x_0,\varepsilon)} |u(x)| \tag{11}$$

and consequently

$$\lim_{\varepsilon \to 0} \varepsilon^{-\delta - (C_1 + C_2\sqrt{E})} \max_{x \in B(x_0,\varepsilon)} |u(x)| = \infty \text{ for all } \delta > 0.$$

The balls are to be taken with respect to the geodesic distance on M.

Remark 2.7.

(i) Even though we did not make any regularity assumption on u, by elliptic regularity theory, see for example [Eva98, Chapter 6.3], we know that any u that solves the eigenvalue equation is in fact in $C^\infty(M)$.

(ii) Vanishing with respect to the $\mathcal{L}^\infty$-norm is a stronger statement than vanishing with respect to the $\mathcal{L}^1$-norm as we have it in the definition of the strong unique continuation property. In fact, let u vanish of order $C_1 + C_2\sqrt{E}$ with respect to the $\mathcal{L}^\infty$-norm. Then we have

$$\int_{B(\varepsilon)} |u(x)| \mathrm{d}x \leq \mathrm{Vol}(B(1)) \cdot \varepsilon^d \max_{x \in B(\varepsilon)} |u(x)| \leq \mathrm{Vol}(B(1)) \cdot \varepsilon^{d + C_1 + C_2\sqrt{E}}.$$

However, for the property of *not vanishing* with respect to some order, the converse implication holds, so that Theorem 2.6 is a weaker statement than one about non-vanishing with respect to the $\mathcal{L}^1$-norm.

Since C_1 and C_2 are not explicitly known, this theorem is most interesting for large E. Inequality (11) controls some kind of local variation of u. The higher E, the larger the variation of u around a point x_0, cf. Example 2.10. It is natural to ask whether one can complement inequality (11) by an upper bound. This has been studied in [DF88] as well.

Definition 2.8. Let $u \in C(M)$ be real-valued. The nodal set of u is $N_u := \{x \in M \mid u(x) = 0\}$. We denote by $\mathcal{H}^{d-1}$ the $(d-1)$-dimensional Hausdorff measure on M.

Recall that eigenfunctions of the Laplacian on an analytic manifold are analytic, see, e.g., [Hör69, Theorem 7.5.1]. By the theory of analytic sets, the nodal sets N_u of such functions have a well-defined Hausdorff measure $\mathcal{H}^{d-1}(N_u)$. The following theorem is due to [DF88, Theorem 1.2].

Theorem 2.9. *Let M be a compact, real-analytic, connected manifold (with real-analytic metric). Then, there exist C_3, C_4, depending on M, such that for every $u : M \to \mathbb{R}$, $0 \not\equiv u$ and every $E \geq 0$ with $-\Delta u = Eu$, we have*

$$C_3\sqrt{E} \leq \mathcal{H}^{d-1}(N_u) \leq C_4\sqrt{E}. \tag{12}$$

Example 2.10 (Vanishing speed and nodal sets of trigonometric functions). Let $M = \mathbb{T}^1 = \mathbb{S}^1 \cong [0,1)$. The eigenfunctions of the Laplace operator on $(0,1)$ with periodic boundary conditions are sin and cos waves. For simplicity we only study the eigenfunctions $u_n(x) = \sin(2\pi n x)$ with corresponding eigenvalue $E_n = (2\pi)^2 n^2$ and their vanishing speed at the point $x = 0$. For ε small, we have

$$2\pi n\varepsilon \geq \sup_{x \in B(\varepsilon)} |u_n(x)| \geq \frac{2\pi n\varepsilon}{2},$$

thus in particular, since ε is small, $\sup_{x\in B(\varepsilon)}|u_n(x)| \geq \varepsilon^{2\pi n} = \varepsilon^{\sqrt{E_n}}$ whence inequality (11) holds with $C_1 = 0$ and $C_2 = 1$. Furthermore, the 0-dimensional Hausdorff measure of the zero set N_{u_n} is the number of zeros of u_n and we have $\mathcal{H}^0(N_{u_n}) = 2n$. Thus, inequality (12) holds with $C_3 = C_4 = 1/\pi$.

Example 2.11 (Vanishing speed and nodal sets of spherical harmonics on $\mathbb{S}^2$). We consider the real part of the spherical harmonics $Y_{l,l}$, $l \in \mathbb{N}$, from Example 1.9, i.e.,

$$\operatorname{Re} Y_{l,l} = \operatorname{Re}\big(c_l \cos(\theta)^l \exp(\mathrm{i}l\phi)\big) = c_l \cos(\theta)^l \cos(l\phi),$$

where $\theta \in [-\pi/2, \pi/2]$ and $\phi \in [0, 2\pi)$. Recall that $-\Delta \operatorname{Re} Y_{l,l} = E_l \operatorname{Re} Y_{l,l}$ where $E_l = l(l+1)$. The function $\operatorname{Re} Y_{l,l}$ exhibits the highest order of vanishing at the poles $\theta = \pm\pi/2$ where its maximum behaves as $|\pm\pi/2 - \theta|^l$. Thus we have for all $x_0 \in \mathbb{S}^2$ and $\varepsilon > 0$ sufficiently small

$$\max_{x \in B(x_0,\varepsilon)} \operatorname{Re} Y_{l,l}(x) \geq \varepsilon^l \geq \varepsilon^{\sqrt{E_l}},$$

where $B(x_0, \varepsilon)$ denotes the ball with center x_0 and radius ε with respect to the geodesic distance. Thus Ineq. (11) of Theorem 2.6 holds with $C_1 = 0$ and $C_2 = 1$.

Concerning Theorem 2.9, we note that the nodal set of $\operatorname{Re} Y_{l,l}$ consists of exactly l meridians. It is of Hausdorff measure $\mathcal{H}^{d-1}(N_{\operatorname{Re} Y_{l,l}}) = 2\pi l$. Hence, Ineq. (12) of Theorem 2.9 is satisfied with $C_3 = \pi$ and $C_4 = 2\pi$.

2.2. A result of Kukavica: Eigenfunctions of Schrödinger operators

Instead of eigenfunctions of the Laplacian, one can study solutions of the stationary Schödinger equation $\Delta u = Vu$ on a manifold M. In this setting the question arises how the vanishing order depends on properties of the potential V.

Next we cite Theorem 5.2 of [Kuk98], which is a generalization of Theorem 2.6.

Theorem 2.12. *Let M be a compact, connected, smooth manifold of dimension d, let $V \in \mathcal{L}^\infty(M)$ and $0 \not\equiv u \in W^{2,2}(M)$ with $\Delta u = Vu$. Then there is a constant $C > 0$, depending only on M, such that u can vanish at most of order*

$$C(1 + \|V\|_\infty^{1/2} + (\operatorname{osc} V)^2),$$

where $\operatorname{osc}(V) := \sup V - \inf V$.

More precisely, for every $x_0 \in M$ and every $\varepsilon > 0$ sufficiently small, we have

$$\varepsilon^{C(1+\|V\|_\infty^{1/2}+(\operatorname{osc} V)^2)} \leq \max_{x \in B(x_0,\varepsilon)} |u(x)|. \tag{13}$$

In the case $V \equiv E$, this theorem reduces to Theorem 2.6. If we choose $V = E \cdot \chi_W$ where χ_W is the characteristic function of a open, non-empty, proper subset $W \subset M$ and E a coupling constant, then the exponent in (13) becomes $C(1+\sqrt{E}+E^2)$, that is quadratic in E. Later, we will see similar statements with the better exponent $C(1 + E^{2/3})$.

Theorems 2.6, 2.9, and 2.12 apply to the d-dimensional torus $\mathbb{T}^d$. This fits nicely to some partial differential equations in Euclidean space. If one considers a cube $\Lambda \subset \mathbb{R}^d$ as a domain and imposes periodic boundary conditions on the solutions of the partial differential equation, then a problem on a torus results. We will come back to discuss this situation in Sections 3.2 and 3.3.

Theorem 2.12 can be reduced (by use of the exponential map) to a statement about elliptic operators on bounded domains $\Omega \subset \mathbb{R}^d$, see [Kuk98] for details.

Theorem 2.13. *Let $\Omega \subset \mathbb{R}^d$ be open, connected and with $C^{1,1}$ boundary. Let $0 \not\equiv u \in W^{2,2}(\Omega)$ satisfy*

$$-\sum_{i,j=1}^{d} \partial_i(a_{ij}\partial_j u) + Vu = 0$$

where $V \in \mathcal{L}^\infty(\Omega)$ and the $a_{ij} \in C^{0,1}(\overline{\Omega})$, $i, j = 1, \ldots, d$ are uniformly Lipschitz continuous functions with $a_{ij} = a_{ji}$, satisfying the following ellipticity condition: there is $\lambda > 0$ such that for all $\xi \in \mathbb{R}^d$ and all $x \in \Omega$ we have

$$|\xi|^2/\lambda \leq \sum_{i,j=1}^{d} a_{ij}(x)\xi_i\xi_j.$$

Furthermore, we assume $|a_{ij}(x)| \leq \lambda$ *and* $|\partial_k a_{ij}(x)| \leq \lambda$ *for almost all* $x \in \overline{\Omega}$ *and that* $a_{ij}|_{\partial\Omega} \in C^{1,1}(\partial\Omega)$, $i, j, k = 1, \dots, d$.

Then there is a constant C*, depending only on* d*,* λ*, the* $C^{1,1}$*-character of* $\partial\Omega$ *and the* $C^{1,1}$*-character of* $a_{i,j}|_{\partial\Omega}$ *such that at every* $x_0 \in \Omega$*,* u *can vanish at most of order* $C(1 + \|V\|_\infty^{1/2} + (\operatorname{osc} V)^2)$.

3. Retrieval of global features from local data

Let $\Lambda \subset \mathbb{R}^d$ be open and connected and $W \subset \Lambda$. One can ask the question whether it is possible to reconstruct certain properties of a function $f : \Lambda \to \mathbb{C}$ only from data or certain features of f on the set W. This might be possible, if one has additional information on the regularity or rigidity of f.

3.1. Rigidity of functions with concentrated Fourier transform

A benchmark for reconstructing functions from partial data is the following theorem which is discussed in detail, e.g., in [BSS88].

Theorem 3.1 (Whittaker–Nyquist–Kotelnikov–Shannon sampling theorem). *Let* $f \in C(\mathbb{R}) \cap \mathcal{L}^2(\mathbb{R})$*, such that the Fourier transform*

$$\hat{f}(p) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{e}^{-ixp} f(x) \mathrm{d}x$$

vanishes outside $[-\pi K, \pi K]$*. Then*

$$(S_K f)(x) = \sum_{j \in \mathbb{Z}} f(j/K) \frac{\sin \pi(Kx - j)}{\pi(Kx - j)}$$

converges absolutely and uniformly on $\mathbb{R}$ *and* $S_K f = f$ *on* $\mathbb{R}$.

One can relax the hypotheses and remove the compact support condition on $\hat{f}$. Then the aliasing error is estimated as

$$\sup_{\mathbb{R}} |f - S_k f| \leq \sqrt{\frac{2}{\pi}} \int_{|p| > \pi K} |\hat{f}(p)| \mathrm{d}p.$$

The Whittaker–Nyquist–Kotelnikov–Shannon sampling theorem allows one to reconstruct the complete function from data on the discrete set $W = \{j/K \mid j \in \mathbb{Z}\} \subset \Lambda = \mathbb{R}$. This is due to the imposed rigidity requirement, which allows only for holomorphic functions. Next we formulate the Logvinenko–Sereda Theorem [LS74], where an upper bound on the $\mathcal{L}^p$-norm of a function is obtained from local data on an appropriately chosen subset $W \subset \mathbb{R}$.

Theorem 3.2 (Logvinenko–Sereda Theorem). *Let* $\gamma, a > 0$*. Let* $W \subset \mathbb{R}$ *be* (γ, a)*-thick, i.e.,* W *is measurable and for all intervals* $I \subset \mathbb{R}$ *of length* a *we have*

$$|W \cap I| \geq \gamma \cdot a.$$

Let $p \in [1,\infty]$, $J \subset \mathbb{R}$ be an interval of length $b > 0$, and $\psi \in \mathcal{L}^p(\mathbb{R})$ with $\hat{\psi}$ supported in J. Then there is a constant $C = C(ab, \gamma)$ such that

$$\|\psi\|_{\mathcal{L}^p(W)} \geq C(ab,\gamma)\|\psi\|_{\mathcal{L}^p(\mathbb{R})}.$$

Note that the constant on the right-hand side does not depend on the position of the interval J, nor on detailed properties of the set W. Here a plays the role of a scale and γ of a density. Logvinenko and Sereda proved the statement with $C(ab,\gamma) = \exp(-c(1+ab)/\gamma)$, while Kovrijkine showed in [Kov01] that the constant $C(ab,\gamma)$ can be chosen as a polynomial $(\gamma/c)^{c(1+ab)}$ of γ. Here c denotes a universal constant independent of the model parameters. Furthermore, he showed the following refinement of the Logvinenko–Sereda Theorem:

Theorem 3.3 (Kovrijkine–Logvinenko–Sereda Theorem). *Let $\gamma, a > 0$. Let $W \subset \mathbb{R}$ be (γ,a)-thick. Let $p \in [1,\infty]$, $J_k \subset \mathbb{R}$, $k = 1,\dots,s$ be intervals of length $b > 0$, and $\psi \in \mathcal{L}^p(\mathbb{R})$ with $\hat{\psi}$ supported in $J = \cup_{k=1}^s J_k$. Then*

$$\|\psi\|_{\mathcal{L}^p(W)} \geq C(ab,\gamma,s,p)\,\|\psi\|_{\mathcal{L}^p(\mathbb{R})}$$

with $C(ab,\gamma,s,p) = (\gamma/c)^{ab(c/\gamma)^s + s - (p-1)/p}$

There exists a multidimensional analog, for $\psi \in \mathcal{L}^p(\mathbb{R}^d)$, of the Logvinenko–Sereda Theorem as well, cf. [Kov01, MS13]. The following consequence of Theorem 3.3 is remarkable.

Corollary 3.4. *Fix $\gamma, a, b > 0, s \in \mathbb{N}$. Let $B\colon \mathcal{L}^2(\mathbb{R}) \to \mathcal{L}^2(\mathbb{R})$ be the multiplication operator with the characteristic function of an (γ,a)-thick set. For an interval J of length b set $\mathcal{F}(J) = \{f \in \mathcal{L}^2(\mathbb{R}) \mid \operatorname{supp}\hat{f} \subset J\}$. While B is not injective, we have*

$$\|\psi\|_{\mathcal{L}^2(\mathbb{R})} \geq \|B\,\psi\|_{\mathcal{L}^2(\mathbb{R})} \geq \left(\frac{\gamma}{c}\right)^{ab(c/\gamma)^s+s-\frac{1}{2}} \|\psi\|_{\mathcal{L}^2(\mathbb{R})} \quad \text{for all } \psi \in \cup +_{k=1}^s \mathcal{F}(J_k) \tag{14}$$

where $+_{k=1}^s\mathcal{F}(J_k) = \operatorname{span}(\mathcal{F}(J_1),\dots\mathcal{F}(J_s))$ and the union runs over all s-tuples $J_1,\dots,J_s \subset \mathbb{R}$ of intervals of length b each.

None of the subspaces $\mathcal{F}(J_k)$ has finite dimension, but they are all unitarily equivalent. The constant c in (14) in particular does not depend on the positions of the intervals J_k. This resembles the definition of the uniform uncertainty principle or restricted isometry property, except for the fact that dimensions of all subspaces are infinite. Let us recall the uniform uncertainty principle, which plays a prominent role in compressed sensing and sparse recovery, cf. for instance [CRT06, FR13].

Definition 3.5. Let $M, n, s \in \mathbb{N}$, $B\colon \mathbb{R}^M \to \mathbb{R}^n$ be a linear map, and $s \leq M$. If

$$(1-\delta_s)\|\psi\|^2 \leq \|B\psi\|^2 \leq (1+\delta_s)\|\psi\|^2$$

for all $\psi \in \mathbb{R}^M$ with $\sharp \operatorname{supp}\psi \leq s$, then δ_s is called a *restricted isometry constant* (for s and B), and B is said to satisfy a *uniform uncertainty principle* or *restricted isometry property*. Here typically $M \gg n$.

While this definition concerns finite matrices, the most interesting situation is when M becomes very large, and one wants an explicit control with respect to the dimension. This setting is then not too far from the infinite-dimensional one. The two-sided inequality (14) may be seen as an instance of the infinite-dimensional analog to Definition 3.5. This and multiscale versions of the Logvinenko–Sereda Theorem will be discussed in detail elsewhere.

Example 3.6 (Spherical harmonics revisited). Let us come back to Example 1.9 of spherical harmonics discussed earlier. In light of the Logvinenko–Sereda Theorem one can also ask the question how one has to choose observation sets $A_L \subset \mathbb{S}^2$, $L \in \mathbb{N}$, such that for all $L \in \mathbb{N}$ one has an observability inequality which is uniform on

$$f \in \mathcal{F}_L = \left\{ f \in \mathcal{L}^2(\mathbb{S}^2) \mid f \in \operatorname{Span} \{ Y_{l,m} \mid l(l+1) < L, -l < m < l \} \right\},$$

that is an inequality

$$\int_{\mathbb{S}^2} |f|^2 \leq C \int_{A_L} |f|^2 \quad \text{for all } f \in \mathcal{F}_L \tag{15}$$

with a constant $C > 1$ that does not depend on L.

The answer is given by Theorem 1 of [OCP13]. We formulate it reduced to the simpler $\mathbb{S}^2$ case.

Theorem 3.7 (Logvinenko–Sereda Theorem on the sphere). *A sequence of sets $A_L \subset \mathbb{S}^2$, $L \in \mathbb{N}$, satisfies* (15) *if and only if there is $r > 0$ such that*

$$\Gamma = \Gamma_r := \inf_{L \in \mathbb{N}} \inf_{z \in \mathbb{S}^2} \frac{\operatorname{vol}\left(A_L \cap B(z, r/\sqrt{L}) \right)}{\operatorname{vol}\left(B(z, r/\sqrt{L}) \right)} > 0.$$

The balls are to be taken with respect to the geodesic distance on $\mathbb{S}^2$.

Here Γ plays the role of a density, while a space scale is provided by $r/\sqrt{L}$. This implies in particular that for (15) to hold, we need that there is $r > 0$ such that for every $L \in \mathbb{N}$ the complement A_L^c contains no $r/\sqrt{L}$-balls.

In the next section we will pursue the question which of the properties discussed so far survive if the class of functions under consideration is not given by a Fourier condition, but by eigenfunctions of Schrödinger operators or linear combinations thereof. This is a natural question, since the expansion in terms of eigenfunctions can be seen as an analogue or generalization of the Fourier transform.

3.2. Eigenfunctions of Schrödinger operators

Recall that for $L > 0$, we write $\Lambda_L = (-L/2, L/2)^d$. We assume that $\Lambda \in \{\mathbb{R}^d, \Lambda_L\}$ and $W \subset \Lambda$ is an equidistributed subset of Λ. To be more precise, given $G, \delta > 0$, we say that a sequence $z_j \in \mathbb{R}^d$, $j \in (G\mathbb{Z})^d$ is (G, δ)-*equidistributed*, if

$$\forall j \in (G\mathbb{Z})^d : \quad B(z_j, \delta) \subset \Lambda_G + j.$$

Corresponding to a (G,δ)-equidistributed sequence z_j we define for $L \in G\mathbb{N}$ the set

$$W_\delta = \bigcup_{j\in(G\mathbb{Z})^d} B(z_j,\delta) \cap \Lambda,$$

see Figure 1 for an illustration. Note that the set W_δ depends on G and the choice of the (G,δ)-equidistributed sequence and, if $\Lambda = \Lambda_L$, also on the scale L. For

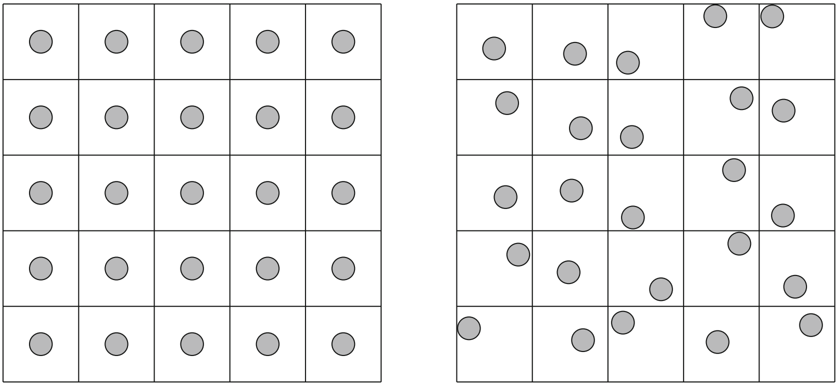

FIGURE 1. Illustration of W_δ within the region $\Lambda = \Lambda_5 \subset \mathbb{R}^2$ for periodically (left) and non-periodically (right) arranged balls.

a bounded and measurable potential $V : \mathbb{R}^d \to \mathbb{R}$ we introduce the self-adjoint Schrödinger operator $H := -\Delta + V$ on $\mathcal{L}^2(\mathbb{R}^d)$. If $\Lambda = \mathbb{R}^d$ then H_Λ coincides with H, if $\Lambda = \Lambda_L$ for some finite L then H_Λ denotes the restriction of $-\Delta + V$ to $\mathcal{L}^2(\Lambda)$ with Dirichlet, Neumann, or periodic boundary conditions. Our aim is to prove $\|\psi\|_{\mathcal{L}^2(W_\delta)} \geq C\|\psi\|_{\mathcal{L}^2(\mathbb{R}^d)}$ for eigenfunctions ψ of H_Λ, with an explicit and L-independent constant $C > 0$. In the one-dimensional situation this problem reduces to an application of Gronwall's inequality as carried out in [Ves96, KV02] for periodically arranged balls on the real line and in [HV07] for balls on metric graphs, cf. Lemma 10 in the preprint [HV06] for details. We restate it here for $(1,\delta)$-equidistributed sequences.

Lemma 3.8. *Let $d = 1$. For each $\delta \in (0, 1/2)$ there is a constant $C_\delta > 0$, such that for all $L \in 2\mathbb{N} - 1$ and $\Lambda \in \{\mathbb{R}, \Lambda_L\}$, $V : \mathbb{R} \to \mathbb{R}$ measurable and bounded, all $\psi \in W^{2,2}(\Lambda)$ satisfying $H_\Lambda\psi = E\psi$ for some $E \in \mathbb{R}$, all $(1,\delta)$-equidistributed sequences z_j, $j \in \mathbb{Z}$, and all $k \in \mathbb{Z} \cap \Lambda$ we have*

$$\|\psi\|_{\mathcal{L}^2(B(\delta,z_k))} \geq C_{\mathrm{ucp}}\|\psi\|_{\mathcal{L}^2(\Lambda_1(k))} \quad \text{and} \quad \|\psi\|_{\mathcal{L}^2(W_\delta)} \geq C_{\mathrm{ucp}}\|\psi\|_{\mathcal{L}^2(\Lambda)},$$

where

$$C_{\mathrm{ucp}} = \left(\lceil 1/\delta \rceil \, \mathrm{e}^{2C_\delta + 2\|V-E\|_\infty}\right)^{-1}.$$

Thus we are indeed considering inequalities of the type (6) as discussed in Remark 1.3.

Proof. For $k \in \Lambda \cap \mathbb{Z}$ set $f_k(x) = \|\psi\|^2_{\mathcal{L}^2(B(x+z_k,\delta))} > 0$ whenever $B(x+z_k,\delta) \subset \Lambda$. By Sobolev norm estimates and the eigenvalue equation there is a δ-dependent constant $C_\delta > 0$ such that

$$\begin{aligned}\left|\frac{\partial}{\partial x} f_k(x)\right| &\leq 2\|\psi\|_{\mathcal{L}^2(B(x+z_k,\delta))}\|\psi'\|_{\mathcal{L}^2(B(x+z_k,\delta))} \\ &\leq 2\left[C_\delta + \|V-E\|_\infty\right]\|\psi\|^2_{\mathcal{L}^2(B(x+z_k,\delta))} = 2\left[C_\delta + \|V-E\|_\infty\right] f_k(x),\end{aligned}$$

see [Ves96, KV02] for details. Applying Gronwall's lemma, we obtain

$$\begin{aligned} & f_k(x) \leq \mathrm{e}^{2[C_\delta + \|V-E\|_\infty]|x|} f_k(0) \\ \Leftrightarrow \quad & \|\psi\|^2_{\mathcal{L}^2(B(x+z_k,\delta))} \leq \mathrm{e}^{2[C_\delta + \|V-E\|_\infty]|x|}\|\psi\|^2_{\mathcal{L}^2(B(z_k,\delta))}. \end{aligned} \tag{16}$$

Positioning $x \in (-1,1)$ we cover $\Lambda_1(k)$ by $\lceil 1/\delta \rceil$ intervals of length δ and obtain

$$\|\psi\|^2_{\mathcal{L}^2(\Lambda_1(k))} \leq \lceil 1/\delta \rceil \, \mathrm{e}^{2C_\delta + 2\|V-E\|_\infty}\|\psi\|^2_{\mathcal{L}^2(B(z_k,\delta))},$$

which proves the first inequality. The second inequality follows immediately by summing up the disjoint intervals $\Lambda_1(k)$, $k \in \mathbb{Z} \cap \Lambda$. □

Note that the constant C_{ucp} in Lemma 3.8 is independent of L. For this reason we call an estimate of this type a scale-free unique continuation principle. The drawback of this result is that it is restricted to the one-dimensional situation. Also, we did not track the explicit δ-dependence.

Now we turn to the multidimensional case. We start by recalling quantitative unique continuation estimates. The following theorem from [BK05] may be understood as an analogue of Theorems 2.6, 2.12, and Ineq. (16) for Schrödinger operators on $\mathbb{R}^d$.

Theorem 3.9. *Let $\gamma, V\colon \mathbb{R} \to \mathbb{R}$ be bounded and measurable, and $u\colon \mathbb{R} \to \mathbb{C}$ a bounded solution of $\Delta u = Vu + \gamma$ with $u(0) = 1$. Then there are constants $c, c' \in (0,\infty)$, such that for all $x \in \mathbb{R}^d$ we have*

$$\max_{|y-x|\leq 1}|u(y)| + \|\gamma\|_\infty > c\exp\left(-c'|x|^{4/3}\log|x|\right). \tag{17}$$

The proof is based on following Carleman estimate, see [EV03, BK05].

Theorem 3.10. *There are $\alpha_0, C > 1$ such that for all $\rho > 0$ there is $w_\rho : \mathbb{R}^d \to \mathbb{R}$ s.t. for all $\alpha \geq \alpha_0$ and $u \in W^{2,2}(\mathbb{R}^d)$ with support in $B(\rho) \setminus \{0\}$ we have*

$$\alpha^3 \int_{\mathbb{R}^d} w_\rho^{-1-2\alpha} u^2 \leq C_1 \rho^4 \int_{\mathbb{R}^d} w_\rho^{2-2\alpha}(\Delta u)^2 \quad \text{and} \quad \frac{|x|}{\mathrm{e}\rho} \leq w_\rho(x) \leq \frac{|x|}{\rho}. \tag{18}$$

Remark 3.11.

(i) In fact one can choose for $\rho > 0$,

$$\begin{aligned} &\varphi\colon [0,\infty) \to [0,\infty), \qquad \varphi(s) := s \cdot \exp\left(-\int_0^s \frac{1-\mathrm{e}^{-t}}{t}\, dt\right), \\ &w_\rho\colon \mathbb{R}^d \to [0,\infty), \qquad w_\rho(x) := \varphi(|x|/\rho). \end{aligned}$$

Then φ is a strictly increasing continuous function, on $(0,\infty)$ even smooth, and

$$\frac{|x|}{\mathrm{e}\rho} \leq w_\rho(x) \leq \frac{|x|}{\rho} \quad \text{for all } x \in B(0,\rho).$$

(ii) The particular feature of this Carleman estimate is that the weight function is not exponential as, e.g., in Ineq. (9). Furthermore, the particular scaling with α is crucial to obtain the exponent $4/3$ in Ineq. (17).

(iii) Theorem 3.9 was a crucial step for the answer on a long-standing problem in the theory of random Schrödinger operators, namely Anderson localization for the continuum Anderson model with Bernoulli-distributed coupling constants. Let us emphasize that the precise decay rate in Ineq. (17) was essential for this application. If, instead of Ineq. (17), one would have at disposal only a slightly weaker version, where the exponent $4/3$ would be replaced by 1.35, one could not conclude localization for the continuum Anderson–Bernoulli model using the same techniques, cf. [BK05, p. 412].

There are local $\mathcal{L}^2$-variants of Theorem 3.9, see [GK13, BK13, RMV13]. As an example, we formulate Theorem 3.4 of [BK13].

Theorem 3.12. *Let $\Lambda \subset \mathbb{R}^d$ be an open subset of $\mathbb{R}^d$ and consider a real measurable and bounded function V on Λ. Let $\psi \in W^{2,2}(\Lambda)$ be real-valued and $\zeta \in \mathcal{L}^2(\Lambda)$ be defined by $-\Delta\psi + V\psi = \zeta$ almost everywhere on Λ. Let $\Theta \subset \Lambda$ be a bounded and measurable set where $\|\psi\|_{\mathcal{L}^2(\Theta)} > 0$. Set*

$$Q(x,\Theta) := \sup_{y\in\Theta}|y-x| \quad \textit{for } x \in \Lambda.$$

Consider $x_0 \in \Lambda \setminus \overline{\Theta}$ such that $Q = Q(x_0,\Theta) \geq 1$, $\operatorname{dist}(x_0,\Theta) > 0$, and $B(x_0, 6Q+2) \subset \Lambda$. Then given $0 < \delta \leq \min\{\operatorname{dist}(x_0,\Theta), 1/24\}$, we have

$$\left(\frac{\delta}{Q}\right)^{K\left(1+\|V\|_\infty^{2/3}\right)\left(Q^{4/3}+\log\frac{\|\psi\|_{\mathcal{L}^2(\Lambda)}}{\|\psi\|_{\mathcal{L}^2(\Theta)}}\right)} \|\psi\|^2_{\mathcal{L}^2(\Theta)} \leq \|\psi\|^2_{\mathcal{L}^2(B(x_0,\delta))} + \delta^2\|\zeta\|^2_{\mathcal{L}^2(\Lambda)}, \tag{19}$$

where $K > 0$ is a constant depending only on d.

Remark 3.13. In the case $\zeta = 0$ inequality (19) estimates the quotient

$$\frac{\|\psi\|_{\mathcal{L}^2(\Theta)}}{\|\psi\|_{\mathcal{L}^2(B(x_0,\delta))}}$$

of two local $\mathcal{L}^2$-norms in terms of another such quotient

$$\frac{\|\psi\|_{\mathcal{L}^2(\Lambda)}}{\|\psi\|_{\mathcal{L}^2(\Theta)}}.$$

If an estimate on the latter is not provided a priori, one might wonder whether one is running in a vicious circle or an induction without induction anchor. Indeed, for many applications the bound in Theorem 3.12, and likewise the corresponding estimates in [GK13, RMV13], need to be complemented by some other information. This is quite analogous with the situation encountered in Example 1.6 and Corollary 1.8. Only when we are supplied with some estimate which controls the global growth of the function f_k, we can say at what fastest rate it can vanish at the origin.

Remark 3.14. Theorem 3.12 is applied in [BK13] to obtain bounds on the density of states outer measure for Schrödinger operators in dimension $d \in \{1,2,3\}$. The restriction on the dimension stems from the decay rate 4/3 in Theorem 3.12 and would be lifted if the inequality (19) would be at disposal with $Q^{4/3}$ replaced by Q. However, in the case of complex-valued potentials Meshkov's example [Mes92] shows that it is not possible to improve the exponent 4/3. The example of Meshkov does not apply to real-valued potentials. However, at the moment it is not known how to exploit this additional property of the potential in order to obtain improved quantitative unique continuation estimates. In particular, an improvement of (19) must be based on some method different from Carleman's estimates.

Let us sketch the basic ideas of the proof of Theorem 3.12 using the Carleman estimate (18).

Sketch of proof of Theorem 3.12. For simplicity, we restrict ourselves to the special case $\zeta \equiv 0$, $\Lambda = \mathbb{R}^d$ and $x_0 = 0$. We cannot apply Ineq. (18) to ψ directly, since ψ is not supported in $B(r) \setminus \{0\}$ for some $r > 0$. Therefore it is natural that a cut off function comes into play. We choose three annuli

$$A_1 = B(3\delta/4) \setminus B(\delta/4), \quad A_2 = B(2\mathrm{e}Q) \setminus B(3\delta/4), \quad A_3 = B(2\mathrm{e}Q+1) \setminus B(2\mathrm{e}Q),$$

and a cutoff function $\eta \in C_0^\infty(\mathbb{R}^d; [0,1])$ as illustrated in Figure 2, with support in $B(2\mathrm{e}Q+1) \setminus B(\delta/4)$ and the properties that

$$\begin{cases} \max\{|\nabla\eta|, |\Delta\eta|\} \leq \tilde{\Theta}_1/\delta^2 =: \Theta_1 & \text{on } A_1, \\ \eta \equiv 1 & \text{on } A_2, \\ \max\{|\nabla\eta|, |\Delta\eta|\} \leq \Theta_2 & \text{on } A_3, \end{cases} \tag{20}$$

for some constants $\tilde{\Theta}_1, \Theta_2 > 0$ which depend only on the dimension. Note that by construction $\Theta \subset A_2 \cap B(Q)$. Now we can apply Ineq. (18) with $\rho = 2\mathrm{e}Q + 2$ to the function $u = \eta\psi$ and obtain using the product rule and $(a+b+c)^2 \leq 3(a^2+b^2+c^2)$ and $|\Delta\psi| = |V\psi|$ that

$$\begin{aligned} \alpha^3 \int_{A_2} w_\rho^{-1-2\alpha} \psi^2 &\leq C_1 \rho^4 \int_{\mathbb{R}^d} w_\rho^{2-2\alpha} (\psi\Delta\eta + \eta\Delta\psi + 2\,(\nabla\eta)^{\mathrm{T}}\,\nabla\psi)^2 \\ &\leq 3C_1\rho^4 \left(\int_{A_1} + \int_{A_2} + \int_{A_3} \right) w_\rho^{2-2\alpha} (\psi^2|\Delta\eta|^2 + \eta^2\|V\|_\infty^2|\psi|^2 + 2|\nabla\eta|^2|\nabla\psi|^2). \end{aligned}$$

Since $w_\rho^{-1} \geq 1$ on A_2 we can replace the weight function on the left-hand side by $w_\rho^{2-2\alpha}$. For the three integrals $\int_{A_i}$, $i \in \{1,2,3\}$, on the right-hand side we proceed as follows. Since $\nabla\eta = \Delta\eta \equiv 0$ and $\eta \equiv 1$ on A_2, we can subsume the second

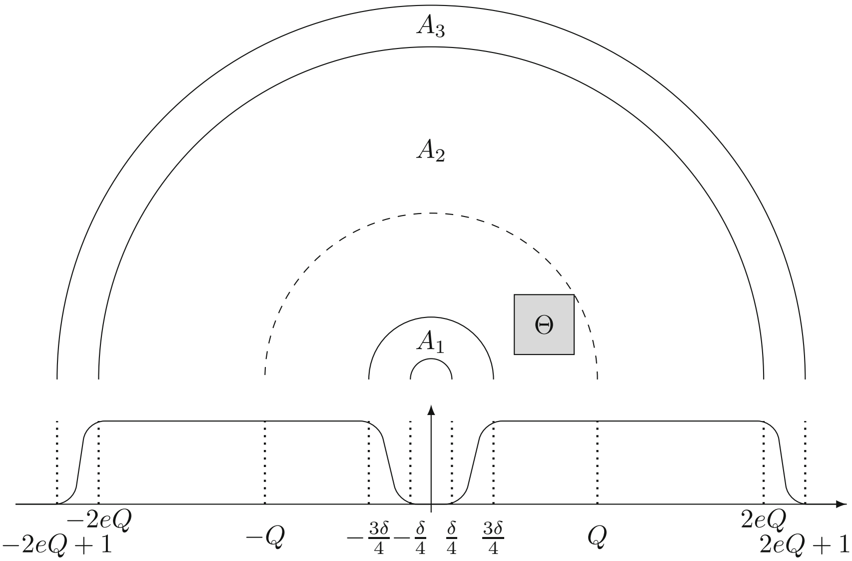

FIGURE 2. Cutoff function η, annuli A_1, A_2, A_3 and the set Θ

integral on the right-hand side into the left-hand side by choosing α sufficiently large. For the first and the third integral we use our bound (20) on the cutoff function and a Cacciopoli inequality to estimate $\int |\nabla\psi|^2$ by a constant (depending on δ and $\|V\|_\infty$) times $\int |\psi|^2$, see, e.g., [BK13] for details. Putting everything together we obtain

$$\alpha^3 \int_{A_2} w_\rho^{2-2\alpha}\psi^2 \lesssim \int_{A_1} w_\rho^{2-2\alpha}\psi^2 + \int_{A_3} w_\rho^{2-2\alpha}\psi^2, \tag{21}$$

up to a multiplicative constant depending on δ, Q, ρ, $\|V\|_\infty$, Θ_1 and Θ_2. Now we use that $\Theta \subset A_2 \cap B(Q)$, $A_1 \subset B(\delta)$ and our bounds on the weight function $(\rho/|x|)^{2\alpha-2} \leq w_\rho^{2-2\alpha}(x) \leq (\mathrm{e}\rho/|x|)^{2\alpha-2}$ on $B(\rho)$ to obtain

$$\alpha^3 \left(\frac{\rho}{Q}\right)^{2\alpha-2} \int_\Theta \psi^2 \lesssim \left(\frac{4\mathrm{e}\rho}{\delta}\right)^{2\alpha-2} \int_{B(\delta)} \psi^2 + \left(\frac{\mathrm{e}\rho}{2\mathrm{e}Q}\right)^{2\alpha-2} \int_\Lambda \psi^2.$$

If

$$\alpha^3 2^{2\alpha} \geq 2\|\psi\|^2_{\mathcal{L}^2(\Lambda)} / \|\psi\|^2_{\mathcal{L}^2(\Theta)},$$

we can subsume $\int_\Lambda \psi^2$ into the left-hand side. The result follows by collecting all the constants. □

Remark 3.15. In Ineq. (21) we estimate the values of the function ψ on the middle annulus A_2 in terms of the values on the inner A_1 and outer A_3 annuli. Thus we have a similar geometric situation as in Hadamard's three circle theorem 1.7.

Quantitative unique continuation estimates as in Theorem 3.12 are useful to obtain scale-free quantitative unique continuation estimates. The following theorem was proven in [RMV13] if $\Lambda = \Lambda_L$ and has been adapted to the case $\Lambda = \mathbb{R}^d$ in [TV15b]. It is a multidimensional analogue of Lemma 3.8 with an explicit dependence on δ and $\|V - E\|_\infty$.

Theorem 3.16. *Let $\Lambda \in \{\Lambda_L, \mathbb{R}^d\}$. There exists a constant $K \in (0, \infty)$ depending merely on the dimension d, such that for any $G > 0$, $\delta \in (0, G/2]$, any (G, δ)-equidistributed sequence z_j, $j \in (G\mathbb{Z})^d$, any measurable and bounded $V : \mathbb{R}^d \to \mathbb{R}$, any $L \in 2\mathbb{N} - 1$ and any real-valued $\psi \in W^{2,2}(\Lambda)$ satisfying $|\Delta\psi| \leq |(V - E)\psi|$ almost everywhere on Λ we have*

$$\|\psi\|_{\mathcal{L}^2(\Lambda_L)} \geq \|\psi\|_{\mathcal{L}^2(W_\delta)} \geq \left(\frac{\delta}{G}\right)^{K(1+G^{4/3}\|V-E\|_\infty^{2/3})} \|\psi\|_{\mathcal{L}^2(\Lambda_L)}. \tag{22}$$

Recall that W_δ denotes the union of δ-balls around an equidistributed sequence. In comparison to Theorem 2.6 we have here no dependence on the diameter of the set Λ_L, because we have not just one base point x_0, but an equidistributed sequence z_j, $j \in (G\mathbb{Z})^d$.

Remark 3.17. Such estimates are called quantitative unique continuation estimates, or uncertainty principles, or observability estimates. Since there is no dependence on $L \in 2\mathbb{N} - 1$ the estimate is called scale-free and the constant $C_{\mathrm{sfuc}} = (\delta/G)^{K_0(1+G^{4/3}\|V-E\|_\infty^{2/3})}$ is called a scale-free unique continuation constant.

The dependence on the other parameters is also of interest. Only the sup-norm $\|V\|_\infty$ of the potential enters, no knowledge of V beyond this is used, in particular no regularity properties. The constant C_{sfuc} is polynomial in δ and (almost) exponential in $\|V\|_\infty$.

Remark 3.18. In order to prove Theorem 3.16 one uses Theorem 3.1 in [RMV13], which is very similar to Theorem 3.12 above. The roles played by the different sets are as follows: Λ is the original finite or infinite cube on which the function ψ is considered. Θ is a cube of side $62\lceil\sqrt{d}\rceil$ centered at a lattice point $k \in \Lambda \cap \mathbb{Z}^d$ inside the cube Λ. One should think of Θ as a neighbourhood of a unit cube $\Lambda_1(k)$ centered at the same k. The ball $B(x_0, \delta)$ is placed in (say the right) next-neighbour unit cube adjacent to $\Lambda_1(k)$. There is an issue with lattice sites k near the boundary of Λ, but for the moment let us consider the case of periodic boundary conditions on the faces Λ. Then we can consider equivalently a partial differential equation on a torus (without boundary). Unfortunately one does not have a priori information about the quotient $\|\psi\|_{\mathcal{L}^2(\Lambda)}/\|\psi\|_{\mathcal{L}^2(\Theta)}$. As discussed before, without this information the bound (19) cannot be applied directly.

It turns out that it is sufficient that the a priori bound holds in a certain averaged sense: not for all lattice points $k \in \Lambda \cap \mathbb{Z}^d$ but just for those which "carry most weight". To make this precise the notion of *dominating sites* is introduced in [RMV13]. One uses the following obvious but useful observation:

Lemma 3.19 (A reverse Markov inequality). *Let $N, T \in \mathbb{N}$ and μ be a probability measure on $\overline{N} := \{1, \dots, N\}$. Set $\mathcal{A} := \{n \in \overline{N} \mid \mu(n) \leq \frac{1}{T}\frac{1}{N}\}$. Then $\mu(A) \leq 1/T$.*

For details of the proof of theorem 3.16 see [RMV13].

Remark 3.20. If we are dealing with neither an eigenfunction ψ, nor a function which satisfies the inequality $|\Delta\psi| \leq |(V - E)\psi|$, but with a linear combinations of eigenfunctions there is no easy way to apply Theorem 3.16. As we will see there are (at least) two approaches how to deal with the problem:

- If the energy interval, which contains the relevant eigenvalues is small enough one can control the norm of ζ sufficiently well. The drawback is that only small energy intervals are allowed.
- Or one uses a more sophisticated argument to exploit the full power of Carleman estimates. This includes introducing an additional ghost dimension and using two different interpolation estimates based on Carleman estimates.

All this will be discussed in the next section.

3.3. Spectral subspaces of Schrödinger operators

In [RMV13] the authors posed the open question whether Ineq. (22) holds also for linear combinations of eigenfunctions, i.e., for $\phi \in \operatorname{Ran} \chi_{(-\infty,E]}(H_\Lambda)$. This is equivalent to

$$\chi_{(-\infty,E]}(H_\Lambda)\, \chi_{W_\delta}\, \chi_{(-\infty,E]}(H_\Lambda) \geq C \chi_{(-\infty,E]}(H_L),$$

with an explicit dependence of C on the parameters δ, E and $\|V\|_\infty$. Here $\chi_I(H_\Lambda)$ denotes the spectral projector of H_Λ onto the interval I. A partial answer, for short energy intervals, was given in [Kle13] in the finite volume case $\Lambda = \{\Lambda_L\}$ and adapted to the case $\Lambda = \mathbb{R}^d$ in [TV15b].

Theorem 3.21. *Let $\Lambda \in \{\mathbb{R}^d, \Lambda_L\}$. There is $K = K(d)$ such that for all $E, G > 0$, $\delta \in (0, G/2)$, all (G, δ)-equidistributed sequences z_j, any measurable and bounded $V\colon \mathbb{R}^d \to \mathbb{R}$, any $L \in 2\mathbb{N} - 1$ and all intervals $I \subset (-\infty, E]$ with*

$$|I| \leq 2\gamma \quad \text{where} \quad \gamma^2 = \frac{1}{2G^4}\left(\frac{\delta}{G}\right)^{K\left(1+G^{4/3}(2\|V\|_\infty+E)^{2/3}\right)},$$

and all $\phi \in \operatorname{Ran} \chi_I(H_\Lambda)$ we have

$$\|\phi\|_{\mathcal{L}^2(W_\delta)} \geq G^4\gamma^2\|\phi\|_{\mathcal{L}^2(\Lambda)}.$$

A full answer to the above question, i.e., Theorem 3.21 for arbitrary compact energy intervals $I \subset \mathbb{R}$ has been given in [NTTV15], while full proofs will be provided in [NTTV].

Theorem 3.22. *Let $\Lambda = \Lambda_L$. There is $K = K(d)$ such that for all $G > 0$, all $\delta \in (0, G/2)$, all (G, δ)-equidistributed sequences z_j, all measurable and bounded $V : \mathbb{R}^d \to \mathbb{R}$, all $L \in G\mathbb{N}$, all $E \geq 0$ and all $\phi \in \operatorname{Ran}(\chi_{(-\infty,b]}(H_{\Lambda_L}))$ we have*

$$\|\phi\|^2_{\mathcal{L}^2(W_\delta)} \geq C_{\mathrm{sfuc}}\|\phi\|^2_{\mathcal{L}^2(\Lambda_L)}$$

where

$$C_{\mathrm{sfuc}} = C_{\mathrm{sfuc}}(d, G, \delta, E, \|V\|_\infty) := \left(\frac{\delta}{G}\right)^{K\left(1+G^{4/3}\|V\|_\infty^{2/3}+G\sqrt{E}\right)}.$$

Let us shortly discuss the ideas for the proof of Theorem 3.22. By scaling it suffices to consider $G = 1$ only. Given $V : \mathbb{R}^d \to \mathbb{R}$ and $L \in \mathbb{N}$ we denote by ψ_k, $k \in \mathbb{N}$, the eigenfunctions of H_{Λ_L} with corresponding eigenvalues E_k. Then given $E \geq 0$ each $\phi \in \mathrm{Ran}(\chi_{(-\infty,E]}(H_{\Lambda_L}))$ can be represented as

$$\phi = \sum_{\substack{k\in\mathbb{N}\\ E_k \leq E}} \alpha_k \psi_k \quad \text{with} \quad \alpha_k = \langle \psi_k, \phi\rangle. \tag{23}$$

Let $R = \lceil 18\mathrm{e}\sqrt{d}\rceil$. Using reflections and translations, we extend the eigenfunctions and the potential $V_L = V|_{\Lambda_L}$ in such a way to Λ_{RL} that the extensions still solve the eigenvalue equation. We use the same symbols V_L and ψ_k for the extended versions. This is possible for periodic, Dirichlet, and Neumann boundary conditions. Let further $F : X = \Lambda_{RL} \times \mathbb{R} \to \mathbb{C}$ be defined by

$$F(x, x_{d+1}) = \sum_{\substack{k\in\mathbb{N}\\ E_k \leq b}} \alpha_k \phi_k(x)\, \mathrm{s}_k(x_{d+1}), \tag{24}$$

where $s_k : \mathbb{R} \to \mathbb{R}$ is given by

$$\mathrm{s}_k(t) = \begin{cases} \sinh(\lambda_k t)/\lambda_k, & E_k > 0,\\ t, & E_k = 0,\\ \sin(\lambda_k t)/\lambda_k, & E_k < 0, \end{cases}$$

with $\lambda_k = \sqrt{|E_k|}$. The function F fulfills

$$\Delta F = \sum_{i=1}^{d+1} \partial_i^2 F = V_L F \quad \text{on} \quad \Lambda_{RL} \times \mathbb{R}$$

and

$$\partial_{d+1} F(\cdot, 0) = \sum_{\substack{k\in\mathbb{N}\\ E_k \leq b}} \alpha_k \psi_k(\cdot) \quad \text{on} \quad \Lambda_{RL}.$$

In particular, for all $x \in \Lambda_L$ we have $\partial_{d+1} F(\cdot, x) = \phi(x)$. This way we recover the original function we are interested in. Let $X_1 = \Lambda_L \times [-1, 1]$ and $X_3 = \Lambda_{L+18\mathrm{e}\sqrt{d}} \times [-9\mathrm{e}\sqrt{d}, 9\mathrm{e}\sqrt{d}]$. The goal is to obtain lower and upper bounds on the H^1-norm of F, more precisely

$$D_1 \|\phi\|_{\mathcal{L}^2(\Lambda_L)} \leq \|F\|_{H^1(X_3)} \leq D_2 \|\phi\|_{\mathcal{L}^2(W_\delta)} \tag{25}$$

with explicit constants D_1 and D_2 independent on the scale L and explicit in all the other parameters. The lower bound is a calculation using the way how the sets Λ_L and X_3 are chosen. For the upper bound we use two different Carleman estimate, namely Ineq. (18) and Proposition 1 in the appendix of [LR95], and conclude two interpolation inequalities for the function F. The two interpolation inequalities read as follows with explicitly controllable constants D_3, D_4 and suitable sets $U_1 \subset U_3 \subset X_3$, see [NTTV] for details on how U_1, U_3 and X_3 are chosen.

Proposition 3.23. *For all* $\delta \in (0, 1/2)$, *all* $(1, \delta)$*-equidistributed sequences* z_j, *all measurable and bounded* $V : \mathbb{R}^d \to \mathbb{R}$, *all* $L \in 2\mathbb{N} - 1$, *all* $E \geq 0$ *and all* ϕ, F *as in* (23) *and* (24) *we have*

$$\|F\|_{H^1(U_1)} \leq D_3 \|(\partial_{d+1}F)(\cdot, 0)\|^{1/2}_{\mathcal{L}^2(W_\delta)} \|F\|^{1/2}_{H^1(U_3)}.$$

Proposition 3.24. *For all* $\delta \in (0, 1/2)$, *all* $(1, \delta)$*-equidistributed sequences* z_j, *all measurable and bounded* $V : \mathbb{R}^d \to \mathbb{R}$, *all* $L \in 2\mathbb{N} - 1$, *all* $E \geq 0$ *and all* ϕ, F *as in* (23) *and* (24) *we have*

$$\|F\|_{H^1(X_1)} \leq D_4 \|F\|^{\gamma}_{H^1(U_1)} \|F\|^{1-\gamma}_{H^1(X_3)}.$$

Let us now show how these two interpolation inequalities are applied to obtain the announced upper bound (25). Again, a calculation shows $\|F\|_{H^1(X_3)} \leq D_5 \|F\|_{H^1(X_1)}$. Applying both interpolation inequalities we conclude

$$\|F\|_{H^1(X_3)} \leq D_5 D_4 D_3 \|F\|^{1-\gamma}_{H^1(X_3)} \|(\partial_{d+1}F)(\cdot, 0)\|^{\gamma/2}_{\mathcal{L}^2(W_\delta)} \|F\|^{\gamma/2}_{H^1(U_3)}.$$

Since $U_3 \subset X_3$ we find

$$\|F\|_{H^1(X_3)} \leq (D_5 D_4 D_3)^{2/\gamma} \|(\partial_{d+1}F)(\cdot, 0)\|_{\mathcal{L}^2(W_\delta)}.$$

Since $\partial_{d+1}F(\cdot, 0) = \phi$ this provides the upper bound and the result follows by estimating carefully all the constants D_i, $i \in \{1, \ldots, 5\}$, and γ.

In a more elementary setting this strategy of proof has been developed already in [JL99]. Additionally, [NTTV] uses ideas from [GK13, RMV13].

4. Applications

4.1. Random Schrödinger operators

This section is concerned with Schrödinger operators with random potential. Such operators serve as quantum mechanical models of disordered condensed matter. Spectral and analytical properties of solutions of corresponding elliptic partial differential equation are studied in order to gain insight in the evolution behaviour of solutions of the corresponding time-dependent Schrödinger equation. This in turn allows for conclusions concerning the transport properties of the modeled material. The most studied type of random Schrödinger operator is the alloy model, also called a continuum Anderson model. We will be concerned with a different type of random operator, namely the random breather model. It is analytically more challenging, due to the non-linear influence of the random variables. In the mathematical literature, random breather potentials have been first considered in [CHM96], and studied in [CHN01] and [KV10]. However, all these papers assumed unnatural regularity conditions, excluding the most basic and standard type of single site potential, where u equals the characteristic function of a ball or a cube. For more details see [NTTV15, NTTV].

Consider a sequence $\omega = (\omega_j)_{j\in\mathbb{Z}^d}$ of positive, independent and identically distributed random variables. We assume that the distribution measure μ of ω_j is supported in an interval $[\omega_-, \omega_+]$ satisfying $0 \leq \omega_- < \omega_+ < 1/2$. The *standard random breather potential* is the function

$$V_\omega(x) = \sum_{j\in\mathbb{Z}^d} \chi_{B(j,\omega_j)}(x),$$

while the family $(H_\omega)_\omega$ with $H_\omega := -\Delta + V_\omega$ on $\mathbb{R}^d$ is called the *standard random breather model*. Note that the random potential is non-negative and uniformly bounded, and thus the operator H_ω is self-adjoint for almost every $\omega \in \Omega$. We also define for $L \in \mathbb{N}$ the operator $H_{\omega,L}$ as the restriction of H_ω onto Λ_L with Dirichlet boundary conditions. $H_{\omega,L}$ is a lower semi-bounded operator with compact resolvent. Hence its spectrum consists of an infinite sequence of (random) isolated eigenvalues of finite multiplicity $E_1^L \leq E_2^L \leq E_3^L \leq \cdots$.

Due to ergodicity the spectrum of the random operator H_ω on the full space is deterministic. This means that there is $\Sigma \subset \mathbb{R}$ such that $\sigma(H_\omega) = \Sigma$, almost surely. Analogous statements hold for the absolutely continuous, the singular continuous, and the pure point part of the spectrum. For most truly random models the singular continuous component of the spectrum is empty, so the prominent question is to determine whether in a certain energy region the Schrödinger operator exhibits pure point or absolutely continuous spectrum, corresponding to localized or delocalized states. A mixture of both types of spectrum in the same energy region would be considered as a physical anomaly. In what we want to discuss, a central quantity is the integrated density of states (IDS) or spectral distribution function $N(E)$. It is a function of the energy and measures the number of energy states per unit volume up to that energy. The definition is as follows:

$$N(E) := \lim_{L\to\infty} \frac{\mathbb{E}\left[\mathrm{Tr}\left[\chi_{(-\infty,E]}(H_{\omega,L})\right]\right]}{L^d}, \quad E \in \mathbb{R}.$$

A priori it is not clear whether the limit exists but in many situations, namely when the family of random operators is ergodic, as is the case here, this is a consequence of ergodic theorems. See the monographs [Sto01, Ves08] for more details and further references.

We are interested in Wegner estimates, that are estimates on the expected number of eigenvalues within an interval $[E-\varepsilon, E+\varepsilon]$ in terms of ε and L^d, the volume of Λ. Such estimates play an important role in proving localization, that is the almost sure existence of pure point spectrum of H_ω near the bottom of Σ. Moreover, our Wegner estimate implies that the integrated density of states is Hölder continuous.

In order to prove a Wegner estimate, we need to understand how the eigenvalues E_n^L, $n \in \mathbb{N}$ of $H_{\omega,L}$ behave if we increase all ω_j by a small amount $\delta > 0$. We use the notation $H_{\omega+\delta,L}$ for the operator $H_{\omega,\delta}$ where all ω_j have been replaced by $\omega_j + \delta$.

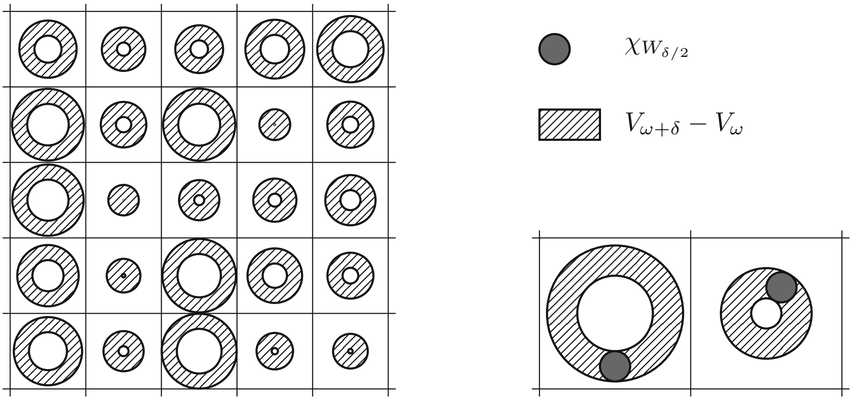

FIGURE 3. Illustration of the increments $V_{\omega+\delta} - V_\omega$ and the choice of $W_{\delta/2}$

Lemma 4.1 (Eigenvalue lifting for the standard random breather model). *Let $H_{\omega,L}$ be as above and assume that $\omega \in [\omega_-, \omega_+]^{\mathbb{Z}^d}$, $\delta \leq 1/2 - \omega_+$. Then, for all $L \in \mathbb{N}$ and all $n \in \mathbb{N}$ with $E_n^L(\omega) \in (-\infty, E_0]$ we have*

$$E_n^L(\omega + \delta) \geq E_n^L(\omega) + \left(\frac{\delta}{2}\right)^{\left[K\left(2+|E_0+1|^{1/2}\right)\right]},$$

where K is the constant from Theorem 3.22. *In particular, K does not depend on L.*

Proof. The function $V_{\omega+\delta} - V_\omega$ is the characteristic function of a disjoint union of annuli each of which has width δ, see Figure 3. Every such annulus contains a ball of radius $\delta/2$, see Figure 3 whence we have $V_{\omega+\delta} - V_\omega \geq \chi_{W_{\delta/2}}$ where $\chi_{W_{\delta/2}}$ is the characteristic function of $W_{\delta/2}$, a union of δ-balls, centered at a $(1,\delta)$-equidistributed sequence. We denote the eigenfunctions, corresponding to $E_i^L(\omega+\delta)$ by ϕ_i^L, $i \in \mathbb{N}$. Since $E_n^L(\omega+\delta) \leq E_n^L(\omega) + 1 \leq E_0 + 1$, we have by Theorem 3.22 for all $\phi \in \operatorname{Span}\{\phi_1, \ldots, \phi_n\}$ with $\|\phi\| = 1$,

$$\left\langle \phi, \chi_{W_{\delta/2,L}} \phi \right\rangle \geq \left(\frac{\delta}{2}\right)^{\left[K\left(2+|E_0+1|^{1/2}\right)\right]}.$$

Using this and the variational characterization of eigenvalues we estimate

$$\begin{aligned} E_n^L(\omega+\delta) &= \langle \phi_n, H_{\omega+\delta,L} \phi_n \rangle \\ &= \max_{\phi \in \operatorname{Span}\{\phi_1,\ldots,\phi_n\}, \|\phi\|=1} \left[\langle \phi, H_{\omega,L}\phi\rangle + \langle \phi, (V_{\omega+\delta,L} - V_{\omega,L})\,\phi\rangle\right] \\ &\geq \max_{\phi \in \operatorname{Span}\{\phi_1,\ldots,\phi_n\}, \|\phi\|=1} \left[\langle \phi, H_{\omega,L}\phi\rangle + \left\langle \phi, \chi_{W_{\delta/2,L}} \phi\right\rangle\right] \end{aligned}$$

$$\geq \inf_{\dim \mathcal{D}=n} \max_{\phi \in \mathcal{D}, \|\phi\|=1} \left[\langle \phi, H_{\omega,L}\phi \rangle + \left(\frac{\delta}{2}\right)^{\left[K\left(2+|E_0+1|^{1/2}\right)\right]} \right]$$
$$= E_n^L(\omega) + \left(\frac{\delta}{2}\right)^{\left[K\left(2+|E_0+1|^{1/2}\right)\right]}. \qquad \square$$

Combining this lemma with the method from [HKN+06] that was developed for random Schrödinger operators with alloy type potential we obtain in [NTTV15, NTTV] a Wegner estimate for the standard random breather model.

Theorem 4.2 (Wegner estimate for the standard random breather model). *Assume that μ has a bounded density ν supported in $[\omega_-, \omega_+]$ with $0 \leq \omega_- < \omega_+ < 1/2$. Fix $E_0 \in \mathbb{R}$. Then there are $C = C(d, E_0)$ and $\varepsilon_{\max} = \varepsilon_{\max}(d, E_0, \omega_+) \in (0, \infty)$ such that for all $\varepsilon \in (0, \varepsilon_{\max}]$ and $E \geq 0$ with $[E - \varepsilon, E + \varepsilon] \subset (-\infty, E_0]$, we have*

$$\mathbb{E}\left[\mathrm{Tr}\left[\chi_{[E-\varepsilon,E+\varepsilon]}(H_{\omega,L})\right]\right] \leq C\|\nu\|_\infty \varepsilon^{[K(2+|E_0+1|^{1/2})]^{-1}} \left|\ln \varepsilon\right|^d L^d$$

where K is the constant from Theorem 3.22. The constant $\varepsilon_{\max}$ can be chosen as

$$\varepsilon_{\max} = \frac{1}{4}\left(\frac{1/2-\omega_+}{2}\right)^{K(2+|E_0+1|^{1/2})}.$$

Here $\mathbb{E}$ denotes the expectation w.r.t. the random variables $\omega_j, j \in \mathbb{Z}^d$. From our Wegner estimate, we can deduce that the IDS is locally Hölder continuous.

Corollary 4.3 (Hölder continuity of the IDS). *For every $E_0 \in \mathbb{R}$ there are constants $\tilde{C}, c > 0$ such that for all $E_1 < E_2 \leq E_0$ we have*

$$|N(E_2) - N(E_1)| \leq C \cdot |E_2 - E_1|^c.$$

Proof. For every $L \in 2\mathbb{N} - 1$ we have

$$\frac{\left|\mathbb{E}\left[\mathrm{Tr}\left[\chi_{(-\infty,E_2]}(H_{\omega,L})\right]\right] - \mathbb{E}\left[\mathrm{Tr}\left[\chi_{(-\infty,E_1]}(H_{\omega,L})\right]\right]\right|}{L^d} \leq \frac{\mathbb{E}\left[\mathrm{Tr}\left[\chi_{[E_1,E_2]}(H_{\omega,L})\right]\right]}{L^d}$$
$$\leq C\|\nu\|_\infty \left|\frac{E_2 - E_1}{2}\right|^{[K(2+|E_0+1|^{1/2})]^{-1}} \cdot \left|\ln \frac{E_2 - E_1}{2}\right|^d$$
$$\leq \tilde{C}|E_2 - E_1|^c. \qquad \square$$

Remark 4.4. In [NTTV, TV15a] we establish the Wegner bound for a much more general class of random potentials. Here, for the sake of simplicity, we have restricted ourselves to the case of the standard random breather model.

In what we presented so far, the scale free unique continuation principle was used to remove the so-called *covering condition*. In fact this condition featured in many older results on Wegner estimates, see for instance the original papers [Kir96, CH94] or the detailed discussion in the monograph [Ves08]. Since the covering conditions plays a role in other types of results on spectral properties of random Schrödinger operators, the scale free unique continuation principle is a promising tool beyond only proofs of Wegner estimates. For instance, results of Shirley [Shi14] on Minami estimates and spectral statistics of one-dimensional models use the covering condition as well. It is natural to conjecture that the scale-free unique continuation principle can be used to remove this assumption. Indeed, this has been carried out in the recent paper [Shi15], see Theorem 1.1 there. It uses the scale-free unique continuation principle of [NTTV15] for one-dimensional configuration space, see [Shi15, Theorem 4.1].

4.2. Control of the heat equation

The aim here is to study in a multiscale geometry the control cost for the heat equation, i.e., the infimum over $\mathcal{L}^2$-norms of control functions which drive a system to zero at a prescribed time $T > 0$.

We consider the controlled heat equation

$$\begin{cases} \partial_t u - \Delta u + Vu = f\chi_W, & u \in \mathcal{L}^2([0,T] \times \Lambda), \\ u = 0, & \text{on } (0,T) \times \partial\Lambda, \\ u(0,\cdot) = u_0, & u_0 \in \mathcal{L}^2(\Lambda), \end{cases} \tag{26}$$

where $\Lambda = \Lambda_L$ is a d-dimensional cube of side length $L \in \mathbb{N}$ and W is a union of δ-balls within Λ, arising from a $(1,\delta)$-equidistributed sequence. In (26) u is the state and f is the control function which acts on the system through the control set $W \subset \Lambda$.

We say that the system (26) is null controllable at time $T > 0$, if there is for each initial state $u_0 \in \mathcal{L}^2(\Lambda)$ a control function $f \in \mathcal{L}^2([0,T] \times W)$ such that the corresponding solution of (26) is zero at time T. It is known, see for instance [FI96], that the system (26) is null controllable at any time $T > 0$. However, we want to estimate the cost, that is the $\mathcal{L}^2$-norm of the control function $f \in \mathcal{L}^2([0,T] \times W)$ in relation to the norm of the initial state u_0.

The controllability cost $\mathcal{C}(T, u_0)$ at time T for the initial state u_0 is given by

$$\mathcal{C}(T, u_0) = \inf \left\{ \|f\|_{\mathcal{L}^2([0,T]\times\omega)} \mid u \text{ is solution of (26) and } u(T,\cdot) = 0 \right\}.$$

Combining Theorem 3.22 with results from [Mil10] one finds the following result, see [NTTV] for details.

Theorem 4.5. *For every $G > 0$, $\delta \in (0, G/2)$ and $K_V \geq 0$ there is*

$$T' = T'(G, \delta, K_V) > 0$$

such that for all $T \in (0, T']$, all (G,δ)-equidistributed sequences, all measurable and bounded $V : \mathbb{R}^d \to \mathbb{R}^d$ with $\|V\|_\infty \leq K_V$ and all $L \in G\mathbb{N}$, the system (26) is null controllable on the set W with cost $\mathcal{C}(T, u_0)$ satisfying

$$\mathcal{C}(T, u_0) \leq 2\sqrt{a_0 b_0} \mathrm{e}^{c_*/T} \|u_0\|_{\mathcal{L}^2(\Lambda)},$$

where

$$\begin{aligned}
a_0 &= (\delta/G)^{-K(1+G^{4/3}\|V\|_\infty^{2/3})},\\
b_0 &= \mathrm{e}^{2\|V\|_\infty},\\
c_* &\leq \ln(G/\delta)^2 \left(KG + 4/\ln 2\right)^2 \quad \textit{and}\\
K &= K(d) \textit{ is the constant from Theorem } 3.22.
\end{aligned}$$

Remark 4.6. The same result holds also in the case of controlled heat equation with periodic or Neumann boundary conditions with obvious modifications.

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