Spectral Inequalities for Discrete and Continuous Differential Operators

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Lukas Wolfgang Schimmer

Department of Mathematics

Imperial College

180 Queen's Gate, London SW7 2AZ

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I certify that this thesis, and the research to which it refers, are the product of my own work, and that any ideas or quotations from the work of other people, published or otherwise, are fully acknowledged in accordance with the standard referencing practices of the discipline.

Lukas Wolfgang Schimmer

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To Lucy.

Abstract

In this thesis spectral inequalities and trace formulae for discrete and continuous differential operators are discussed.

We first investigate spectral inequalities for Jacobi operators with matrix-valued potentials and present a new, direct proof of a sharp inequality corresponding to a Lieb–Thirring inequality for the power $3/2$ using the commutation method. For the special case of a discrete Schrödinger operator we also prove new inequalities for higher powers of the eigenvalues and the potential and compare our results to previously established bounds.

We then approximate a Schrödinger operator on $L^2(\mathbb{R})$ by Jacobi operators on $\ell^2(\mathbb{Z})$ and use the established inequalities to provide new proofs of sharp Lieb–Thirring inequalities for the powers $\gamma = 1/2$ and $\gamma = 3/2$. By means of interpolation we derive spectral inequalities for Jacobi operators that yield (non-sharp) Lieb–Thirring constants on the real line for powers $1/2 < \gamma < 3/2$.

We then consider Schrödinger operators on a finite interval $[0, b]$ with matrix-valued potential and establish trace formulae of the Buslaev–Faddeev–Zakharov type. The results link sums of powers of the negative eigenvalues to terms dependent on the potential and scattering functions.

Finally, we discuss the Berezin inequality, which is well-known on sets of finite measure and find an analogous inequality for the magnetic operator with constant magnetic field on a set whose complement has finite measure. We obtain a similar bound for the Heisenberg sub-Laplacian.

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Table of Symbols

$\mathbb{N}$	The set of natural numbers
$\mathbb{Z}$	The set of integers
$\mathbb{R}$	The set of real numbers
$\mathbb{C}$	The set of complex numbers
$\mathrm{Re}\, a$	The real part of a complex number a
$\mathrm{Im}\, a$	The imaginary of a complex number a
$\overline{a}$	The complex conjugate of a complex number a
A^*	The adjoint of an operator A
$\mathrm{tr} A$	The trace of an operator A
$\det A$	The determinant of a matrix A
$\mathbb{I}$	The identity operator
$\mathcal{C}^\infty$	The set of infinitely differentiable functions
$\mathcal{C}_c^\infty$	The set of infinitely differentiable functions with compact support
ℓ^p	The set of sequences for which the p-th power of the absolute value is summable
L^p	The set of functions for which the p-th power of the absolute value is integrable
$\Gamma(x)$	The Gamma function
$\mathrm{B}(x, y)$	The Beta function

Chapter 1

Introduction

The research conducted in this thesis concentrates on trace formulae and spectral inequalities in the field of discrete and continuous differential operators. The thesis is based on [64, 65] as well as unpublished work. The results of this work expand on already established identities and inequalities for the Schrödinger operator and generalise them to other differential operators, such as the Jacobi operator, which are of interest in their own right. Some of the established results will in turn be used to derive results for the Schrödinger operator, in particular in the context of approximating the continuous differential operator by discrete operators.

To this end the Schrödinger operator H will be introduced in the next section. In the following sections the trace identities and trace inequalities for H, which are generalised in this thesis, will be discussed. In Section 1.4 an overview of the research in this thesis will be given. Chapters 2, 3, 4 and 5 will present in detail the work conducted in this thesis.

1.1 The Schrödinger Operator

The Schrödinger operator H is defined as

$$H := \begin{cases} \operatorname{dom}(H) \subset L^2(\Omega) \to L^2(\Omega)\,, \\ (H\psi)(x) = (-\Delta\psi)(x) + V(x)\psi(x)\,, \end{cases} \tag{1.1}$$

where Ω is an open subset of $\mathbb{R}^d$ and $-\Delta = -\sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2}$ denotes the d-dimensional Laplacian. The real-valued function V is referred to as the potential. The domain of H is chosen in such a way that the operator becomes self-adjoint. This involves imposing not only reg-

ularity conditions on the functions in $\mathrm{dom}(H)$ but in some cases also boundary conditions. The spectrum of the Schrödinger operator H depends heavily on the choice of boundary conditions as well as the dimension d, the set Ω and the potential V.

A more general definition considers H on $L^2(\Omega, \mathcal{H})$, the space of square-integrable functions with values in a separable Hilbert space $\mathcal{H}$. In this setting the potential $V(x)$ is a self-adjoint operator on $\mathcal{H}$ for all $x \in \Omega$. This is not merely an abstract generalisation of H but proves to be a fruitful approach in the investigation of higher-dimensional Schrödinger operators, as we will explain briefly in Section 1.3. In this thesis the cases $\Omega = \mathbb{R}, \mathcal{H} = \mathbb{C}$ and $\Omega = [0, b] \subseteq \mathbb{R}, \mathcal{H} = \mathbb{C}^m$ with Dirichlet boundary conditions will be considered.

Our main interest lies in the negative part of the spectrum of H. Defining the positive/negative part of a self-adjoint operator A as $A_\pm = \frac{1}{2}(|A| \pm A)$, we shall consider $H_- = (-\Delta + V)_-$. The so-called Riesz means are defined as the traces $\mathrm{tr}(-\Delta + V)_-^\gamma$ for $\gamma \geq 0$ and provide an effective tool in the investigation of the negative spectrum of H. Note that, a-priori, it is not clear whether these traces exist, i.e. whether the operators $(-\Delta + V)_-^\gamma$ are trace-class. For illustrational purposes, we note that if the negative spectrum of H consists of a finite number of eigenvalues $\mu_1, \ldots, \mu_N$, then it holds that $\mathrm{tr}(-\Delta + V)_-^\gamma = \sum_{j=1}^N |\mu_j|^\gamma$.

Riesz means have been studied extensively in the literature. Firstly there are explicit identities which express $\mathrm{tr}(-\Delta + V)_-^\gamma$ in terms of the potential and certain functions originating from scattering theory. A brief overview of established results will be provided in Section 1.2. Secondly, it is possible to give upper and lower bounds on the Riesz means. Ideally, these bounds depend in a simple way only on known characteristics of H such as the potential V, the set Ω and the dimension d. The most important results will be summarised in Section 1.3.

1.2 Trace Formulae

In general, trace formulae relate the spectrum of H to characteristics of the operator itself. The first trace formula for Schrödinger operators was proved in 1953 by Gel′fand and Levitan [33]. In their work the authors considered the operator (1.1) for $d = 1$ and Ω a compact interval which they chose to be $\Omega = [0, \pi]$ without loss of generality. With Dirichlet boundary conditions $\psi(0) = \psi(\pi) = 0$ the spectrum of the differential operator H is found to be discrete, consisting solely of a countable number of eigenvalues μ_j, $j \in \mathbb{N}$. These eigenvalues can be arranged such that they tend to infinity, i.e. $\lim_{j\to\infty} \mu_j = \infty$. In

the special case of a vanishing potential, $V \equiv 0$, the eigenvalues can be calculated explicitly as $\mu_{j,0} = j^2$. Gel′fand and Levitan proved that, under the assumption $\int_0^\pi V(x)\,\mathrm{d}x = 0$, the identity

$$\sum_{j=1}^{\infty}(\mu_j - \mu_{j,0}) = -\frac{1}{4}\big(V(0) + V(\pi)\big) \tag{1.2}$$

holds. The right-hand side can be identified as the regularised trace of the differential operator, which will be explained in more detail in Section 4.4. The remarkable property of (1.2) is that the left-hand side, which contains all the eigenvalues of H, can be simply computed by evaluating the potential at the two endpoints.

This result inspired a number of authors and has led to many new results in the case $d = 1$. In [23] regularised trace formulae for all integer powers of the eigenvalues μ_j were proved. Later, singular operators defined on the half-line were considered by Buslaev and Faddeev [12]. The object of their interest was the Schrödinger operator H on $\Omega = [0, \infty)$ with Dirichlet boundary condition at the origin. The potential V is assumed to be continuous and short-range, which means that it is integrable and its first moment $\int_0^\infty xV(x)\,\mathrm{d}x$ is finite. In this setting the continuous spectrum coincides with the positive real axis and the negative part of the spectrum consists of a finite number of discrete eigenvalues $\mu_1, \dots, \mu_N$. In their work, Buslaev and Faddeev found expressions for the trace of the negative part of integer and half-integer powers of the differential operator H. The first two trace formulae read

$$\begin{aligned}
\operatorname{tr}\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V\right)_-^{\frac{1}{2}} &= \sum_{j=1}^{N} |\mu_j|^{\frac{1}{2}} = \frac{1}{\pi}\int_0^{+\infty} \log a(\zeta)\,\mathrm{d}\zeta - \frac{1}{4}\int_0^{+\infty} V(x)\,\mathrm{d}x, \\
\operatorname{tr}\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V\right)_- &= \sum_{j=1}^{N} |\mu_j| \;\; = \frac{2}{\pi}\int_0^{+\infty} \zeta\left(\eta(\zeta) - \frac{1}{2\zeta}\int_0^{+\infty} V(x)\,\mathrm{d}x\right)\mathrm{d}\zeta + \frac{1}{4}V(0),
\end{aligned} \tag{1.3}$$

where $a(\zeta)$ is the so-called limit amplitude and $\eta(\zeta)$ the limit phase. Both originate from scattering theory and for their exact definition we refer to the literature (e.g. [77]). Their meaning will become clearer in Chapter 4. In [77] a second proof of these identities can be found as well as an analogous result for the Schrödinger operator on the real line, $\Omega = \mathbb{R}$. In [22] the half-line problem with Robin boundary condition at the origin was studied. The results in both of these cases take a similar form to (1.3). The case of long-range potentials

on the half-line was treated in [62, 4].

Identities of the form (1.3) are henceforth referred to as Buslaev–Faddeev–Zakharov trace formulae. While most of the aforementioned trace identities are of this type, we note that there are also results which resemble (1.2) in their form, for example for the perturbed harmonic oscillator [56]. These regularised trace formulae emerge when the spectrum consists of an infinite number of eigenvalues.

The trace identities have found a number of interesting applications. They play an important role in numerous papers on inverse scattering theory, such as [21, 3] to name only a few. They have also been used to characterise the absolutely continuous spectrum in the case of square-integrable potentials on the real line [20]. In this case, the trace identity corresponding to the power $5/2$ has been used to prove that the Korteweg–de Vries equation is completely integrable [28].

In recent years some of these trace identities have been adapted to a more general setting where the operator (4.1) is defined on $L^2(\Omega, \mathcal{H})$, the space of square-integrable functions with values in a separable Hilbert space $\mathcal{H}$. In this setting the potential $V(x)$ is required to be a self-adjoint operator on $\mathcal{H}$ for all $x \in \Omega$. In the case of $\mathcal{H} = \mathbb{C}^m$ the operator H corresponds to a system of differential equations.

Identity (1.2) was generalised to the case of $\mathcal{H}$ being a separable Hilbert space in [39]. The formula was also generalised to star-shaped graphs [78]. In [47] Laptev and Weidl considered the case $\mathcal{H} = \mathbb{C}^m$, $\Omega = \mathbb{R}$, where the negative spectrum consists of a finite number of eigenvalues $\mu_1, \dots, \mu_N$ each with a multiplicity $m_j \leq m$. In complete analogy to the scalar result [77] the authors obtained the trace formulae for half-integer powers. The first two can be written as

$$\begin{aligned}
\operatorname{tr}\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V\right)_-^{\frac{1}{2}} &= \sum_{j=1}^{N} m_j |\mu_j|^{\frac{1}{2}} = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \log a(\zeta)\,\mathrm{d}\zeta - \frac{1}{4}\int_{-\infty}^{+\infty} \operatorname{tr} V(x)\,\mathrm{d}x\,, \\
\operatorname{tr}\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V\right)_-^{\frac{3}{2}} &= \sum_{j=1}^{N} m_j |\mu_j|^{\frac{3}{2}} = -\frac{3}{2\pi}\int_{-\infty}^{+\infty} \zeta^2 \log a(\zeta)\,\mathrm{d}\zeta + \frac{3}{16}\int_{-\infty}^{+\infty} \operatorname{tr} V(x)^2\,\mathrm{d}x.
\end{aligned} \tag{1.4}$$

While this result was proved for $d = 1$, the authors were able to deduct from it a Lieb–Thirring inequality that applies to any dimension $d \geq 1$. The applied method will be discussed briefly in the next subsection.

1.3 Trace Inequalities

We present an overview of two types of spectral inequality that provide bounds on Riesz means of the Schrödinger operator.

1.3.1 Lieb–Thirring Inequalities

Lieb–Thirring inequalities were first introduced by Lieb and Thirring [53]. The authors considered the Schrödinger operator (1.1) on $\Omega = \mathbb{R}^d$ and showed that if $\gamma > \max(0, 1-\frac{d}{2})$ there exists a constant $L_{\gamma,d}$ such that

$$\operatorname{tr}(-\Delta + V)_-^\gamma \leq L_{\gamma,d} \int_{\mathbb{R}^d} V(x)_-^{\gamma+\frac{d}{2}} \, \mathrm{d}x \,. \tag{1.5}$$

The proof of Lieb and Thirring uses the Birman–Schwinger kernel [9, 67]. Subsequently the inequality was extended to the case $\gamma = 0$, $d \geq 3$ [16, 50, 60], where it is known as the Cwikel–Lieb–Rozenblum bound. The remaining critical case $\gamma = \frac{1}{2}$, $d = 1$, was proved to hold by Weidl [74].

Sharp Constants

It is an interesting problem to identify the value of the sharp constant $L_{\gamma,d}$. The semi-classical Lieb–Thirring constant $L^{\mathrm{cl}}_{\gamma,d}$ is defined as

$$L^{\mathrm{cl}}_{\gamma,d} = (4\pi)^{-\frac{d}{2}} \frac{\Gamma(\gamma+1)}{\Gamma(\gamma+1+\frac{d}{2})}$$

and it emerges in the semi-classical approximation, which goes back to the beginning of quantum mechanics. We consider the phase space of points $(p, x) \in \mathbb{R}^{2d}$. The momentum operator $-\mathrm{i}\nabla$ is identified with p and we assume that every quantum state is supported in a volume of size $(2\pi)^d$ in the phase space. Then the approximation

$$\sum_{j\geq 1} |\mu_j|^\gamma \approx \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \left(p^2 + V(x)\right)_-^\gamma \, \mathrm{d}p \, \mathrm{d}x = L^{\mathrm{cl}}_{\gamma,d} \int_{\mathbb{R}^d} V(x)_-^{\gamma+\frac{d}{2}} \, \mathrm{d}x$$

is derived. Note that this computation holds for all values of $\gamma > 0$.

A Weyl-type asymptotic result implies that the semi-classical approximation becomes

exact in the limit of large coupling, i.e. that for sufficiently smooth V

$$\lim_{\eta\to\infty} \frac{1}{\eta^{\gamma+\frac{d}{2}}} \mathrm{tr}(-\Delta + \eta V)_-^\gamma = L^{\mathrm{cl}}_{\gamma,d} \int_{\mathbb{R}^d} V(x)_-^{\gamma+\frac{d}{2}} \,\mathrm{d}x\,.$$

This immediately yields that $L^{\mathrm{cl}}_{\gamma,d} \leq L_{\gamma,d}$ for all $\gamma \geq \max(0, 1-\frac{d}{2})$. In investigating whether these two constants are equal, the trace formulae mentioned in the previous subsection play an important role. Lieb and Thirring [53] were able to show that $L^{\mathrm{cl}}_{\gamma,d} = L_{\gamma,d}$ in the case $\gamma \geq \frac{3}{2}$, $d = 1$. Their proof is based on the Buslaev–Faddeev–Zakharov trace formulae for Schrödinger operators on $\mathbb{R}$ and the observation that the limit-amplitude satisfies $a(\zeta) \geq 1$ for $\zeta \in \mathbb{R}$. The Aizenman–Lieb principle [2] established that for fixed dimension $d \geq 1$ the ratio $L_{\gamma,d}/L^{\mathrm{cl}}_{\gamma,d}$ is a monotonic, non-increasing function of γ. Laptev and Weidl [47] were able to show that $L_{\gamma,d} = L^{\mathrm{cl}}_{\gamma,d}$ in the case $\gamma \geq \frac{3}{2}$, $d \geq 1$. From their trace formula (1.4) the authors deducted that for a Schrödinger operator with matrix-valued potential the inequality

$$\mathrm{tr}\,(-\Delta + V)_-^\gamma \leq L^{\mathrm{cl}}_{\gamma,d} \int_{-\mathbb{R}^d} \mathrm{tr}\Big(V(x)_-^{\gamma+\frac{d}{2}}\Big)\,\mathrm{d}x \tag{1.6}$$

holds in the special case of $\gamma = \frac{3}{2}, d = 1$ as long as the right-hand side is finite. It was an essential observation that this inequality is also true in the more general case where the Schrödinger operator is defined on functions taking values in a separable Hilbert space. Inequality (1.6) was then extended to $\gamma \geq \frac{3}{2}$ using the Aizenman–Lieb principle, and by an induction argument making use of the underlying Hilbert space, the inequality was shown to hold for any $d \geq 1$, which implied the desired result $L^{\mathrm{cl}}_{\gamma,d} = L_{\gamma,d}$. More recently Stubbe [72] provided a new proof of the sharp constant for $\gamma \geq 2, d \geq 1$, by means of a monotonicity argument with respect to coupling constants.

For $\gamma = \frac{1}{2}$, $d = 1$, Hundertmark, Lieb and Thomas [41] showed that the best constant is given by $L_{1/2,1} = 2L^{\mathrm{cl}}_{1/2,1} = \frac{1}{2}$ and that the inequality is sharp for delta potentials in this case. For $1 \leq \gamma < \frac{3}{2}$ it was proved in [25] that the sharp constant can be bounded from above by $L_{\gamma,1} \leq \frac{\pi}{\sqrt{3}} L^{\mathrm{cl}}_{\gamma,1}$, which was subsequently generalised to higher dimension in [24]. In the scalar case Lieb and Thirring [53] conjectured that for $\frac{1}{2} < \gamma < \frac{3}{2}$ the sharp constant is given by

$$L_{\gamma,1} = 2L^{\mathrm{cl}}_{\gamma,1} \left(\frac{\gamma - \frac{1}{2}}{\gamma + \frac{1}{2}}\right)^{\gamma-\frac{1}{2}}.$$

Kinetic Energy Inequalities and the Stability of Matter

The importance of the sharp values of $L_{\gamma,d}$ lies in their relation to the ground state energy of matter. As proved in [53] the Lieb–Thirring inequality (1.5) for $\gamma = 1$ is equivalent to the lower bound

$$\sum_{i=1}^{N} \int_{\mathbb{R}^d} |\nabla_i \psi|^2 \, \mathrm{d}x_i \geq \frac{K_d}{||\gamma_\psi^{(1)}||_\infty^{(1+2/d)/(1+d/2)}} \int_{\mathbb{R}^d} \rho_\psi(x)^{1+\frac{2}{d}} \, \mathrm{d}x \tag{1.7}$$

on the kinetic energy of a normalised N-particle wave function $\psi \in L^2(\mathbb{R}^{Nd})$. Here, ρ_ψ denotes the one-body density ($x \in \mathbb{R}^d$)

$$\rho_\psi(x) = \sum_{i=1}^{N} \int_{\mathbb{R}^{(N-1)d}} |\psi(x_1, \dots, x_{i-1}, x, x_{i+1}, \dots, x_N)|^2 \, \mathrm{d}x_1 \cdots \mathrm{d}x_{i-1} \, \mathrm{d}x_{i+1} \cdots \mathrm{d}x_N$$

and $||\gamma_\psi^{(1)}||_\infty \leq N$ is the largest eigenvalue of the one-particle density matrix, which is an operator on $L^2(\mathbb{R}^d)$ defined by the kernel ($x, x' \in \mathbb{R}^d$)

$$\gamma_\psi^{(1)}(x, x') = \sum_{i=1}^{N} \int_{\mathbb{R}^{(N-1)d}} \psi(x_1, \dots, x_{i-1}, x, x_{i+1}, \dots, x_N) \overline{\psi}(x_1, \dots, x_{i-1}, x', x_{i+1}, \dots, x_N) \cdot \mathrm{d}x_1 \cdots \mathrm{d}x_{i-1} \, \mathrm{d}x_{i+1} \cdots \mathrm{d}x_N \, .$$

The sharp constant K_d is related to the sharp constant $L_{1,d}$ via

$$\left(\left(1 + \frac{2}{d} \right) K_d \right)^{1+\frac{d}{2}} \left(\left(1 + \frac{d}{2} \right) L_{1,d} \right)^{1+\frac{2}{d}} = 1 \, .$$

In essence, (1.7) gives a lower bound on the kinetic energy necessary to create a density ρ_ψ with N particles in d dimensions. As shown later [61], the kinetic energy inequality (1.7) (with a smaller constant) can also be proved directly, without the use of the Lieb–Thirring inequality.

This inequality was instrumental in the proof of stability of matter as presented in [53]. (see also [52]). The sharp value of $L_{1,d}$ is important to obtain precise bounds on the ground state energy of a system of electrons and nuclei interacting via the Coulomb force. Furthermore, if $L_{1,3} = L_{1,3}^{\mathrm{cl}}$ were proved to be true, the lower bound (1.7) would be the kinetic energy term in Thomas–Fermi theory (see e.g. [51]).

1.3.2 The Berezin Inequality

The semi-classical Lieb–Thirring constants $L^{\mathrm{cl}}_{\gamma,d}$ also emerge in a different spectral inequality. Let Ω be an open subset of $\mathbb{R}^d$ such that its measure $|\Omega|$ is finite. In [7] Berezin proved that the Dirichlet Laplacian $-\Delta^{\mathcal{D}}$ on Ω satisfies the inequality

$$\operatorname{tr}(-\Delta^{\mathcal{D}} - \mu)^{\gamma}_{-} \leq (2\pi)^{-d}|\Omega| \int_{\mathbb{R}^d} (|p|^2 - \mu)^{\gamma}_{-} \, \mathrm{d}p = L^{\mathrm{cl}}_{\gamma,d}|\Omega|\mu^{\gamma+\frac{d}{2}} \tag{1.8}$$

for all $\mu \geq 0$, $\gamma \geq 1$. The constant $L^{\mathrm{cl}}_{\gamma,d}$ is sharp, which follows from an asymptotic result by Weyl [75]. For the inequality to hold it is essential that the Laplace operator is considered on the set Ω of finite volume. This guarantees that H only has discrete spectrum consisting of eigenvalues converging to infinity, showing that the left-hand side of (1.8) exists.

The Berezin inequality (1.8) has inspired a number of authors and is related to the Li–Yau inequality [48]. In their paper the authors showed that the sum over the first k eigenvalues $\mu_1, \ldots, \mu_k$ of $-\Delta^{\mathcal{D}}$ on Ω can be bounded from below as

$$\sum_{j=1}^{k} \mu_j \geq \frac{d}{d+2} \big(L^{\mathrm{cl}}_{0,d}|\Omega|\big)^{-\frac{2}{d}} k^{\frac{d+2}{d}} .$$

This was later proved to be a corollary of (1.8) via the Legendre transformation [46]. In [45] comparable inequalities were established for various classes of differential and pseudo-differential operators including $((-\Delta)^{\alpha})^{\mathcal{D}}$ with $\alpha > 0$. A similar inequality to (1.8) can also be found for Schrödinger operators with magnetic fields in the case $d = 2$. The operator $H^{\mathcal{D}}_B := (-\mathrm{i}\nabla + A(x))^2$ on $L^2(\Omega)$ with Dirichlet boundary conditions and arbitrary vector field A satisfies

$$\operatorname{tr}(H^{\mathcal{D}}_B - \mu)^{\gamma}_{-} \leq L^{\mathrm{cl}}_{\gamma,2}\mu^{\gamma+1}|\Omega| \tag{1.9}$$

for all $\gamma \geq \frac{3}{2}$, which follows from a result by Laptev and Weidl [47] (see also [30]). In [26] this was generalised to $\gamma \geq 1$ under the restriction that the magnetic field $B = \mathrm{d}A$ is a positive constant. The upper bound in (1.9) can then be improved by allowing it to depend

on B

$$\operatorname{tr}(H_B^{\mathcal{D}} - \mu)_-^\gamma \leq |\Omega| \frac{B}{2\pi} \sum_{k=0}^{\infty} \big((2k+1)B - \mu\big)_-^\gamma \tag{1.10}$$

as shown in [30]. In their paper the authors also proved that under the assumption that Ω is a tiling domain this inequality also holds if $0 \leq \gamma < 1$, where it is sharp. For $\gamma = 1$ the right-hand side of (1.10) can be adapted to magnetic operators with additional external potentials V [31]. The Berezin inequality was furthermore extended to the sub-Laplacian L on the Heisenberg group $\mathbb{H}^1$. In [40] (see also [71]), it was proved that the Dirichlet realisation $L^{\mathcal{D}}$ of L on a domain $\Omega \subset \mathbb{H}^1$ of finite measure satisfies

$$\operatorname{tr}(L^{\mathcal{D}} - \mu)_-^\gamma \leq |\Omega| \frac{1}{16} \frac{1}{(\gamma+1)(\gamma+2)} \mu^{\gamma+2} . \tag{1.11}$$

1.4 Overview and Summary of Results

In Chapter 2 we will discuss Lieb–Thirring inequalities for Jacobi operators. The content of this chapter was published in [65].

[65] L. Schimmer. Spectral inequalities for Jacobi operators and related sharp Lieb–Thirring inequalities on the continuum. *Comm. Math. Phys.*, to appear, http://dx.doi.org/10.1007/s00220-014-2137-3, 2014.

The main results of Chapter 2 are Theorems 2.2.1, 2.2.2 and 2.2.3. The first theorem provides an inequality corresponding to a Lieb–Thirring inequality for the power $3/2$ for the Jacobi operator on $\ell^2(\mathbb{Z})$. The second theorem generalises this result to Jacobi operators with matrix-valued potentials. While these two inequalities are not new, we will provide new, direct proofs for them in Sections 2.3 and 2.4 by means of the commutation method. Theorem 2.2.3 then establishes previously unknown inequalities for higher powers of the eigenvalues and the potential of the Jacobi operator. The proof will be given in Section 2.5. Subsequently the sharpness of all the established inequalities will be discussed in Section 2.6.

In Chapter 3 we will investigate the approximation of a Schrödinger operator on $L^2(\mathbb{R})$ by Jacobi operators on $\ell^2(\mathbb{Z})$. Using the inequalities of Chapter 2 we will provide new proofs of the sharp Lieb–Thirring constants $L_{1/2,1}$ and $L_{3/2,1}$ on the continuum. In Section 3.1 we will see that in order to obtain the sharp $L_{3/2,1}$ it is not sufficient to restrict the

approximating operators to discrete Schrödinger operators. In Section 3.2 we will show how the sharp constant can be obtained by using Jacobi operators with non-trivial off-diagonal entries. For this reason, the new inequalities of Theorem 2.2.3, which we managed to prove only for discrete Schrödinger operators, will not yield the sharp Lieb–Thirring constants $L_{\gamma,1}$ on $L^2(\mathbb{R})$. The results of the first two sections were published in [65]. Using a symmetry argument we will show in Section 3.3 that the sharp constant $L_{3/2,1}$ can also be obtained through approximation by Jacobi operators with vanishing potentials. In Section 3.4 we will interpolate between a result by Hundertmark and Simon [42] and the result of Theorem 2.2.1 to obtain spectral inequalities for Jacobi operators corresponding to Lieb–Thirring inequalities for powers $1/2 < \gamma < 3/2$. Approximation will then yield (non-sharp) Lieb–Thirring constants $L^{**}_{\gamma,1}$ on the continuum.

In Chapter 4 we will discuss trace formulae for the Schrödinger operator (1.1) on a compact set $\Omega = [0, b] \subseteq \mathbb{R}$. We will consider the more general case of a matrix-valued potential such that H is defined on $L^2([0, b], \mathbb{C}^m)$. The main result will be Theorem 4.3.3, which yields trace formulae of the Buslaev–Faddeev–Zakharov type for the operator under consideration. The inequalities are similar to (1.3) and (1.4). The proof will be based on an asymptotic expansion of a matrix-valued Wronskian. We will also discuss the relevance of this expansion to the regularised trace formula (1.2).

Chapter 5 is based on [64], where the Berezin inequality on domains of infinite measure is discussed.

[64] L. Schimmer. The Berezin inequality on domains of infinite measure. *Bull. Math. Sci.*, 3(1):173–182, 2013.

The main results are Theorem 5.1.3 and Theorem 5.1.4, which are stated in Section 2.2. The first theorem considers the two-dimensional magnetic Schrödinger operator with constant magnetic field and contains a similar bound to (1.10). The second theorem investigates the Heisenberg sub-Laplacian and provides a bound similar to (1.11). The statements require the introduction of a regularised trace.

In Appendix A the copyright information regarding the papers [64, 65] will be provided.

Chapter 2

Spectral Inequalities for Jacobi Operators

The research in this chapter was published in [65]. The self-adjoint Jacobi operator W on $\ell^2(\mathbb{Z})$ is defined as

$$(Wu)(n) = a(n-1)u(n-1) + a(n)u(n+1) + b(n)u(n), \quad n \in \mathbb{Z}\,. \tag{2.1}$$

The sequence $a : \mathbb{Z} \to \mathbb{R}^-$ is assumed to be negative with $\lim_{|n|\to\infty} a(n) = -1$. Motivated by the representation of W as a doubly infinite matrix, the numbers $a(n)$ are referred to as the off-diagonal entries of W. The potential $b : \mathbb{Z} \to \mathbb{R}$ is supposed to be real-valued with $\lim_{|n|\to\infty} b(n) = 0$. We will sometimes use the notation $W_{a,b}$ to emphasise the sequences a and b in the definition of the Jacobi operator. If $a(n) = -1$ for all $n \in \mathbb{Z}$ we call W a discrete Schrödinger operator. Note that, when aiming to obtain sharp Lieb–Thirring inequalities on the continuum, it is not sufficient to consider only discrete Schrödinger operators on $\ell^2(\mathbb{Z})$ to approximate Schrödinger operators on $L^2(\mathbb{R})$. As we shall see later, it is essential to derive spectral inequalities for general off-diagonal entries $a(n)$ which are not constant -1. The only exception is the case $\gamma = \frac{1}{2}$. Below we will give a brief overview of known spectral inequalities for Jacobi operators and explain how our results relate to them.

2.1 Lieb–Thirring Inequalities for Jacobi Operators

Let the numbers $|\lambda_1| > |\lambda_2| > \cdots \geq 2$ denote the (not necessarily finite) sequence of eigenvalues of W outside the essential spectrum $[-2, 2]$, arranged by decreasing modulus. These eigenvalues are all simple (see e.g. [73, Lemma 3.6]). Hundertmark and Simon [42] proved that

$$\sum_{j\geq 1} \left(|\lambda_j|^2 - 4\right)^{\frac{1}{2}} \leq \sum_{n\in\mathbb{Z}} |b(n)| + 4 \sum_{n\in\mathbb{Z}} |a(n) + 1| \tag{2.2}$$

provided that the right-hand side is finite. The authors first established the inequality in the special case of discrete Schrödinger operators by using a modified version of the Birman–Schwinger principle as introduced in [41]. In complete analogy to the case of a Schrödinger operator on the continuum, the inequality was proved to be sharp for delta potentials. Hundertmark and Simon then used a perturbation argument to extend the result to more general off-diagonal entries $a(n)$. As this argument will become important later, we repeat it briefly here. The key observation is that

$$\begin{pmatrix} -|a(n)+1| & -1 \\ -1 & -|a(n)+1| \end{pmatrix} \leq \begin{pmatrix} 0 & a(n) \\ a(n) & 0 \end{pmatrix} \leq \begin{pmatrix} |a(n)+1| & -1 \\ -1 & |a(n)+1| \end{pmatrix}$$

which can be proved easily by considering the trace and the determinant of the difference of respective sides of the inequalities. As a consequence the operator inequalities

$$W_{-1,b^-} \leq W_{a,b} \leq W_{-1,b^+}$$

hold, where the potentials $b^\pm$ are defined as

$$b^\pm(n) = b(n) \pm \left(|a(n-1)+1| + |a(n)+1|\right).$$

The Min–Max principle (see e.g. [59, Theorem XIII.1]) and (2.2) for W_{-1,b^-} then imply that the negative eigenvalues λ_j^- of $W_{a,b}$ satisfy

$$\begin{aligned} \sum_{j\geq 1} (|\lambda_j^-|^2 - 4)^{\frac{1}{2}} &\leq \sum_{n\in\mathbb{Z}} \left(b(n) - |a(n-1)+1| - |a(n)+1|\right)_- \\ &\leq \sum_{n\in\mathbb{Z}} b(n)_- + 2\sum_{n\in\mathbb{Z}} |a(n)+1|. \end{aligned}$$

A similar result can be proved for the positive eigenvalues of $W_{a,b}$ with the help of W_{-1,b^+} and adding the two inequalities yields (2.2). The constants in front of the two sums on the right-hand side (1 and 4) were both found to be optimal.

To obtain analogous inequalities to (2.2) for higher powers of the eigenvalues, Hundertmark and Simon applied the Aizenman–Lieb principle [2] which requires the inequality to be written in terms of $\operatorname{dist}(\lambda_j, [-2,2]) = |\lambda_j| - 2$. This can be done using $|\lambda_j|^2 - 4 \geq 4(|\lambda_j| - 2)$ and for powers $\gamma \geq \frac{1}{2}$ it yields the Lieb–Thirring inequalities

$$\sum_{j\geq 1} \big(|\lambda_j| - 2\big)^\gamma \leq c_\gamma \left(\sum_{n\in\mathbb{Z}} |b(n)|^{\gamma+\frac{1}{2}} + 4 \sum_{n\in\mathbb{Z}} |a(n)+1|^{\gamma+\frac{1}{2}} \right) \tag{2.3}$$

with the constants

$$c_\gamma = 3^{\gamma-\frac{1}{2}} \frac{1}{2} \frac{\Gamma(\gamma+1)\Gamma(2)}{\Gamma(\gamma+\frac{3}{2})\Gamma(\frac{3}{2})} \,.$$

In the special case where $a \equiv -1$, the constant c_γ can be replaced by the smaller value $d_\gamma = 3^{\frac{1}{2}-\gamma} c_\gamma$. This stems from the fact that Hundertmark and Simon again first established the inequalities for discrete Schrödinger operators and then used the aforementioned perturbation argument together with the convexity result

$$\begin{aligned} &\big(b(n) - |a(n-1)+1| - |a(n)+1|\big)_-^{\gamma+\frac{1}{2}} \\ &\leq 3^{\gamma-\frac{1}{2}} \big(b(n)_-^{\gamma+\frac{1}{2}} + |a(n-1)+1|^{\gamma+\frac{1}{2}} + |a(n)+1|^{\gamma+\frac{1}{2}}\big) \end{aligned}$$

to extend them to more general off-diagonal entries $a(n)$. As shown later in [63], the constants c_γ and d_γ can be improved by a factor $\frac{\pi}{2\sqrt{3}}$ if $\gamma \geq 1$. If we let $\eta > 0$ and consider W with a potential ηb then the ratio of the left-hand side to the right-hand side of (2.2) converges to 1 as $\eta \to \infty$. In (2.3), however, the left-hand side grows like η^γ, whereas the right-hand side behaves like $\eta^{\gamma+\frac{1}{2}}$, suggesting that the bounds are not optimal for large eigenvalues.

Hundertmark and Simon [42] used the inequality $(\lambda_j)^2 - 4 \geq (|\lambda_j| - 2)^2$ and the Aizenman–Lieb principle to show that (2.2) also implies

$$\sum_{j\geq 1} \big(|\lambda_j| - 2\big)^{\gamma+\frac{1}{2}} \leq 3^{\gamma-\frac{1}{2}} \left(\sum_{n\in\mathbb{Z}} |b(n)|^{\gamma+\frac{1}{2}} + 4 \sum_{n\in\mathbb{Z}} |a(n)+1|^{\gamma+\frac{1}{2}} \right) \tag{2.4}$$

where $\gamma \geq \frac{1}{2}$. If $a(n) = -1$ for all $n \in \mathbb{Z}$, the factor $3^{\gamma-\frac{1}{2}}$ can be omitted. Inequality (2.4) has the desired property that for potentials ηb the ratio of the left-hand side to the right-hand side converges to 1 as $\eta \to \infty$. It is, however, not optimal for small coupling. In fact, for eigenvalues close to the essential spectrum, the left-hand side of inequality (2.3) is much larger than the left-hand side of (2.4), while the corresponding right-hand sides only differ by a multiplicative constant. Only (2.2) is optimal for both large and small coupling. Note that in [42] the inequalities (2.3) and (2.4) were also generalised to matrix-valued potentials and hence, by applying the method developed by Laptev and Weidl [47], also to d-dimensional Jacobi operators.

To obtain optimal estimates for both small and large coupling, different types of inequalities have to be introduced. Killip and Simon [44] showed that if we write the eigenvalues as $\lambda_j = -k_j - \frac{1}{k_j}$ with $|k_j| > 1$, then

$$\sum_{j\geq 1} \left(k_j^2 - \frac{1}{k_j^2} - \log |k_j|^4 \right) \leq \sum_{n\in\mathbb{Z}} b(n)^2 + 2 \sum_{n\in\mathbb{Z}} \left(a(n)^2 - 1 - \log a(n)^2 \right) . \tag{2.5}$$

Note the emergence of logarithmic terms on both sides of this inequality. The term $\log |k_j|^4$ is essential to guarantee good estimates for both small and large coupling, as we will discuss later.

In their paper [44], Killip and Simon derived (2.5) from an identity obtained from Case's sum rules (first stated in [14]), for which they provided two different proofs. The first proof made use of the perturbation determinant and the Jost function of W and yielded sum rules for Jacobi operators on $\ell^2(\mathbb{N})$ and on $\ell^2(\mathbb{Z})$. The second proof only considered the half-line case $\ell^2(\mathbb{N})$ and involved a continuous fraction expansion of the m-function. Killip and Simon used the sum rules not only to show (2.5) but also to prove a characterisation of Hilbert–Schmidt perturbations of the free Jacobi operator and results related to the Szegő condition. Using the same methods, (2.5) was generalised to matrix-valued potentials B in [68]. Note that, for the case of a discrete Schrödinger operator, inequality (2.5) can also be found in earlier work by Deift and Killip [20]. In their paper, the inequality is obtained from a trace identity for W.

In this thesis, we will provide a new, direct proof of (2.5), without the use of Case's sum rules. To do so, we will apply the commutation method, which goes back to the idea of inserting eigenvalues into the spectrum of differential operators as discussed by Jacobi [43], Darboux [18] and Crum [15]. For more details on this method and some of its applications

we refer to [19] and [34] as well as [35], which specifically considers the case of Jacobi operators. The commutation method was used in [66] where the Schmincke inequality was established for a Schrödinger operator on $L^2(\mathbb{R})$. The same method can also be applied to Schrödinger operators with matrix-valued potentials. Benguria and Loss [5] presented an elementary proof of sharp Lieb–Thirring inequalities for Schrödinger operators on the continuum with matrix-valued potentials based on the commutation method. This provided a new proof of the inequality that had previously been established using trace identities (1.4) by Laptev and Weidl [47]. Similar results were obtained on the half-line in [27]. In this thesis we will also consider matrix-valued potentials, providing a new proof for the analogous inequality to (2.5) in this more general setting. As shown in [55] the commutation method can furthermore be used to prove trace inequalities for higher powers of the eigenvalues of a Schrödinger operator on $L^2(\mathbb{R})$. We will, however, not apply this approach to Jacobi operators in this thesis.

This chapter is organised as follows. In Section 2.2 we will state our main results for scalar Jacobi operators as well as for the case of matrix-valued potentials. In the subsequent sections the proofs of these statements are given. We will aim to make a connection between (2.2) and (2.5). We will show in Section 2.5 that, at least in the case of a discrete Schrödinger operator, the latter can be obtained from the former using an adaptation of the Aizenman–Lieb principle. This is especially interesting as both inequalities are optimal for large coupling. In contrast, a similar argument in the case of a Schrödinger operator on the continuum does not allow us to deduce the optimal Lieb–Thirring inequality for $\gamma = \frac{3}{2}$ from the case of $\gamma = \frac{1}{2}$. Using the adapted Aizenman–Lieb principle, we will also prove new inequalities for discrete Schrödinger operators for any $\gamma \geq \frac{1}{2}$. These inequalities will include logarithmic terms, and we will prove in Section 2.6 that they are more precise than (2.3) and (2.4). In Section 2.6 it will also be shown that inequality (2.5) is sharp for an explicit choice of W with reflectionless potential. For all known non-trivial reflectionless potentials it holds that $a \not\equiv -1$, leading to the conclusion that in contrast to (2.2) the inequality does not necessarily have an optimiser when restricted to discrete Schrödinger operators.

2.2 Statement of the Main Results

We assume that $a(n)$ and $b(n)$ are both uniformly bounded for $n \in \mathbb{Z}$ such that (2.1) defines a self-adjoint operator W with domain $\ell^2(\mathbb{Z})$.

Theorem 2.2.1 *Assume that* $\sum_{n\in\mathbb{Z}} \big(a(n)^2 - 1 - \log a(n)^2\big)$ *is finite and* $b \in \ell^2(\mathbb{Z})$. *Then it holds that*

$$\sum_{j\geq 1} \left(k_j^2 - \frac{1}{k_j^2} - \log|k_j|^4\right) \leq \sum_{n\in\mathbb{Z}} b(n)^2 + 2\sum_{n\in\mathbb{Z}} \big(a(n)^2 - 1 - \log a(n)^2\big) \tag{2.6}$$

and this inequality is sharp. In particular, the discrete Schrödinger operator with $a(n) = -1$ *for all* $n \in \mathbb{Z}$ *and square-summable potential* b *satisfies*

$$\sum_{j\geq 1} \left(k_j^2 - \frac{1}{k_j^2} - \log|k_j|^4\right) \leq \sum_{n\in\mathbb{Z}} b(n)^2 \,.$$

A proof of the first part of this theorem based on the commutation method will be given in Section 2.3. A similar result can be shown to hold for Jacobi operators with matrix-valued potentials. On $\ell^2(\mathbb{Z}, \mathbb{C}^m)$ we consider the operator

$$(Wu)(n) = A(n-1)^* u(n-1) + A(n)u(n+1) + B(n)u(n), \tag{2.7}$$

where the off-diagonal entries $A(n) \in \mathbb{C}^{m\times m}$ are invertible matrices for all $n \in \mathbb{Z}$ and the potential $B(n) \in \mathbb{C}^{m\times m}$ is Hermitian. We furthermore assume that $A(n) \to -\mathbb{I}$ as $|n| \to \infty$ and that $\|A(n)\|$ and $\|B(n)\|$ are uniformly bounded for $n \in \mathbb{Z}$. The latter guarantees that the operator W is well-defined on the domain $\ell^2(\mathbb{Z}, \mathbb{C}^m)$, where it can be shown to be self-adjoint. In the special case of $A \equiv -\mathbb{I}$ we call W a discrete Schrödinger operator with matrix-valued potential. For a survey on Jacobi operators with matrix-valued potentials we refer to [17]. Let $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq 2$ be the eigenvalues of W outside of $[-2, 2]$, arranged by decreasing modulus. For each eigenvalue λ_j the multiplicity is denoted by $m_j \leq m$ and the numbers $|k_j| > 1$ are defined as above.

Theorem 2.2.2 *Assume that* $\sum_{n\in\mathbb{Z}} \big(\mathrm{tr}(A(n)A(n)^* - \mathbb{I}) - \log\det(A(n)A(n)^*)\big)$ *is finite and* $\mathrm{tr}(B^2) \in \ell^1(\mathbb{Z})$. *Then it holds that*

$$\begin{aligned} &\sum_{j\geq 1} m_j \left(k_j^2 - \frac{1}{k_j^2} - \log|k_j|^4\right) \\ &\leq \sum_{n\in\mathbb{Z}} \mathrm{tr}\big(B(n)^2\big) + 2\sum_{n\in\mathbb{Z}} \Big(\mathrm{tr}\big(A(n)A(n)^* - \mathbb{I}\big) - \log\det\big(A(n)A(n)^*\big)\Big) \end{aligned} \tag{2.8}$$

and this inequality is sharp. In particular, the discrete Schrödinger operator with $A(n) =$

$-\mathbb{I}$ *for all* $n \in \mathbb{Z}$ *and* $\operatorname{tr}(B^2) \in \ell^1(\mathbb{Z})$ *satisfies*

$$\sum_{j\geq 1} m_j \left(k_j^2 - \frac{1}{k_j^2} - \log |k_j|^4 \right) \leq \sum_{n\in\mathbb{Z}} \operatorname{tr}\big(B(n)^2\big) \,. \tag{2.9}$$

Here and in the remainder of this chapter the trace is taken in $\mathbb{C}^m$.

Adapting the Aizenman–Lieb principle [2], we also prove spectral inequalities which depend on higher powers of the eigenvalues λ_j and the potential B. These results are only obtained for discrete Schrödinger operators, $A \equiv -\mathbb{I}$. Here, $\mathrm{B}(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}$ denotes the Beta function.

Theorem 2.2.3 *Let* W *be the discrete Schrödinger operator* (2.7) *with* $A(n) = -\mathbb{I}$ *for all* $n \in \mathbb{Z}$*. Enumerate the eigenvalues outside of* $[-2,2]$ *as* $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq 2$ *with multiplicities* $m_j \leq m$*. Then it holds that for* $\gamma > \frac{1}{2}$

$$\sum_{j\geq 1} m_j \int_2^{|\lambda_j|} (E^2-4)^{\frac{1}{2}} (|\lambda_j| - E)^{\gamma - \frac{3}{2}} \,\mathrm{d}E \leq \mathrm{B}\left(\gamma - \frac{1}{2}, 2\right) \sum_{n\in\mathbb{Z}} \operatorname{tr}\left(|B(n)|^{\gamma+\frac{1}{2}} \right) \tag{2.10}$$

provided that the right-hand side is finite. Defining $|k_j| \geq 1$ *via* $\lambda_j = -k_j - \frac{1}{k_j}$*, this inequality coincides for* $\gamma = \frac{3}{2}$ *with* (2.9)*. For* $\gamma = \frac{5}{2}$ *and* $\gamma = \frac{7}{2}$ *the inequality can be written as*

$$\begin{aligned}
&\sum_{j\geq 1} m_j \left(\frac{3}{2} \left(|k_j| - \frac{1}{|k_j|} \right) + \frac{1}{6} \left(|k_j|^3 - \frac{1}{|k_j|^3} \right) - \log |k_j|^2 \left(|k_j| + \frac{1}{|k_j|} \right) \right) \\
&\leq \frac{1}{6} \sum_{n\in\mathbb{Z}} \operatorname{tr}\left(|B(n)|^3 \right) , \\
&\sum_{j\geq 1} m_j \left(\frac{1}{12} \left(k_j^4 - \frac{1}{k_j^4} \right) + \frac{7}{3} \left(k_j^2 - \frac{1}{k_j^2} \right) - \log |k_j|^2 \left(k_j^2 + \frac{1}{k_j^2} \right) - \log |k_j|^6 \right) \\
&\leq \frac{1}{12} \sum_{n\in\mathbb{Z}} \operatorname{tr}\left(|B(n)|^4 \right) .
\end{aligned}$$

2.3 Proof of Theorem 2.2.1

For the moment, we shall assume that the potential b vanishes if $|n|$ is large enough, i.e. $b(n) = 0$ for $|n| > n_{\max}$. We also assume that $a(n) = -1$ for $|n| > n_{\max}$. Under these assumptions the Jacobi operator W has a finite number of eigenvalues outside of $[-2,2]$,

which we denote by

$$\lambda_1 < \cdots < \lambda_L < -2 < 2 < \lambda_{L+1} < \cdots < \lambda_M \,.$$

Here, we have slightly changed the enumeration of the eigenvalues such that the first L eigenvalues are negative and the rest positive. Each of the λ_j can be written uniquely as $\lambda_j = -k_j - \frac{1}{k_j}$, where $|k_j| \geq 1$.

2.3.1 Elimination of Negative Eigenvalues

Let φ be the eigenfunction to the lowest eigenvalue λ_1, i.e. the solution to the equation $W\varphi = \lambda_1\varphi$. Let us assume that $\lambda_1 < -2$, so that $k_1 > 1$. For $n < -n_{\max}$ the eigenequation $W\varphi = \lambda_1\varphi$ takes a very simple form,

$$-\varphi(n-1) - \varphi(n+1) = \lambda_1\varphi(n)\,.$$

It is easy to verify that a complete set of solutions of this equation is spanned by the functions k_1^n and k_1^{-n}. Since $\varphi \in \ell^2(\mathbb{Z})$ and $k_1 > 1$ we conclude that $\varphi(n) = ck_1^n$ for $n < -n_{\max}$. Similarly we can treat the case $n > n_{\max}$ and we can describe the behaviour of φ for sufficiently large or small n as

$$\varphi(n) = \begin{cases} ck_1^n, & n < -n_{\max} \\ dk_1^{-n}, & n > n_{\max} \end{cases} \tag{2.11}$$

with constants $c, d \in \mathbb{R}$. These constants can be chosen in such a way that $\varphi(n) > 0$, which follows from the fact that $(W - \lambda_1) \geq 0$ (see e.g. [37, Theorem 2.8]).

Following [35] we now introduce the operator D on $\ell^2(\mathbb{Z})$ as

$$(Du)(n) = -\sqrt{\frac{-a(n)\varphi(n)}{\varphi(n+1)}}u(n+1) + \sqrt{\frac{-a(n)\varphi(n+1)}{\varphi(n)}}u(n)$$

and note that its adjoint is given by

$$(D^*u)(n) = -\sqrt{\frac{-a(n-1)\varphi(n-1)}{\varphi(n)}}u(n-1) + \sqrt{\frac{-a(n)\varphi(n+1)}{\varphi(n)}}u(n)\,.$$

The eigenequation $W\varphi = \lambda_1\varphi$ can be written as

$$a(n-1)\frac{\varphi(n-1)}{\varphi(n)} + a(n)\frac{\varphi(n+1)}{\varphi(n)} = \lambda_1 - b(n)\,, \tag{2.12}$$

which can be used to show that $D^*D = W - \lambda_1$. This identity allows us to conclude that the spectrum of the operator D^*D coincides with the spectrum of W, shifted by $-\lambda_1$. In particular, the eigenvalues of D^*D are $0, \lambda_2 - \lambda_1, \ldots, \lambda_M - \lambda_1$. We also consider the operator DD^*, which can be written as $DD^* = W_1 - \lambda_1$ where W_1 is a Jacobi operator given by

$$(W_1 u)(n) = a_1(n-1)u(n-1) + a_1(n)u(n+1) + b_1(n)u(n)\,,$$

with off-diagonal entries

$$a_1(n) = -\frac{\sqrt{a(n)a(n+1)\varphi(n)\varphi(n+2)}}{\varphi(n+1)} \tag{2.13}$$

and potential

$$b_1(n) = -a(n)\left(\frac{\varphi(n)}{\varphi(n+1)} + \frac{\varphi(n+1)}{\varphi(n)}\right) + \lambda_1\,. \tag{2.14}$$

Note that $a_1(n) = -1$ and $b_1(n) = 0$ if $|n|$ is sufficiently large. A general result (see e.g. [19]) shows that the operators D^*D and DD^* have the same spectrum with the possible exception of the eigenvalue zero. Assume that there exists a non-vanishing function ψ such that $DD^*\psi = 0$. It follows that $D^*\psi = 0$ and as a consequence, for $n < -n_{\max}$, it must hold that

$$-\sqrt{\frac{1}{k_1}}\psi(n-1) + \sqrt{k_1}\psi(n) = 0\,.$$

Multiplying this equation by $\sqrt{k_1}$ we find that $\psi(n) = pk_1^{-n}$ with $p \in \mathbb{R}$. This function is only in $\ell^2(-\mathbb{N})$ if $p = 0$, which implies that ψ vanishes everywhere. Consequently zero is not an eigenvalue of DD^*. Thus the Jacobi operator W_1 has precisely the eigenvalues $\lambda_2, \ldots, \lambda_M$. We now aim to express $\sum_{n\in\mathbb{Z}} b_1(n)^2$ in terms of k_1 and the potential b. To this

end we recall (2.14) and compute that

$$\begin{aligned}&\sum_{n\in\mathbb{Z}} b_1(n)^2\\&= \sum_{n\in\mathbb{Z}}\left(a(n)^2\left(\frac{\varphi(n)}{\varphi(n+1)}+\frac{\varphi(n+1)}{\varphi(n)}\right)^2-2\lambda_1 a(n)\left(\frac{\varphi(n)}{\varphi(n+1)}+\frac{\varphi(n+1)}{\varphi(n)}\right)+\lambda_1^2\right).\end{aligned} \tag{2.15}$$

Note that the summands vanish if $|n|$ is sufficiently large, say if $|n| > N$. This allows us to write all the involved series as finite sums and reorder as we please. Using (2.12) we can compute that

$$\begin{aligned}&\sum_{n=-N}^{N} a(n)\left(\frac{\varphi(n)}{\varphi(n+1)}+\frac{\varphi(n+1)}{\varphi(n)}\right)\\&= \sum_{n=-N+1}^{N+1} a(n-1)\frac{\varphi(n-1)}{\varphi(n)}+\sum_{n=-N}^{N} a(n)\frac{\varphi(n+1)}{\varphi(n)}\\&= a(N)\frac{\varphi(N)}{\varphi(N+1)}-a(-N-1)\frac{\varphi(-N-1)}{\varphi(-N)}+\sum_{n=-N}^{N}\big(\lambda_1-b(n)\big).\end{aligned}$$

The two terms outside the sum can be calculated by recalling that choosing N sufficiently large guarantees that $a(N) = a(-N-1) = -1$. From (2.11) we then obtain

$$\sum_{n=-N}^{N} a(n)\left(\frac{\varphi(n)}{\varphi(n+1)}+\frac{\varphi(n+1)}{\varphi(n)}\right) = -k_1+\frac{1}{k_1}+\sum_{n=-N}^{N}\big(\lambda_1-b(n)\big). \tag{2.16}$$

To treat the remaining terms in (2.15) we consider the square of equation (2.12). This

allows us to establish that

$$\begin{aligned}
&\sum_{n=-N}^{N} a(n)^2 \left(\frac{\varphi(n)^2}{\varphi(n+1)^2} + \frac{\varphi(n+1)^2}{\varphi(n)^2} \right) \\
&= \sum_{n=-N+1}^{N+1} a(n-1)^2 \frac{\varphi(n-1)^2}{\varphi(n)^2} + \sum_{n=-N}^{N} a(n)^2 \frac{\varphi(n+1)^2}{\varphi(n)^2} \\
&= a(N)^2 \frac{\varphi(N)^2}{\varphi(N+1)^2} - a(-N-1)^2 \frac{\varphi(-N-1)^2}{\varphi(-N)^2} \\
&\quad + \sum_{n=-N}^{N} \left(\big(\lambda_1 - b(n)\big)^2 - 2a(n)a(n-1) \frac{\varphi(n-1)\varphi(n+1)}{\varphi(n)^2} \right).
\end{aligned}$$

Note that the second factor in the sum on the right-hand side equals $2a_1(n-1)^2$ and using (2.11) once again, as well as $a(N) = a(-N-1) = -1$, we obtain the identity

$$\begin{aligned}
&\sum_{n=-N}^{N} a(n)^2 \left(\frac{\varphi(n)^2}{\varphi(n+1)^2} + \frac{\varphi(n+1)^2}{\varphi(n)^2} \right) \\
&= k_1^2 - \frac{1}{k_1^2} + \sum_{n=-N}^{N} \left(\big(\lambda_1 - b(n)\big)^2 - 2a_1(n-1)^2 \right).
\end{aligned} \tag{2.17}$$

Inserting (2.16) and (2.17) into (2.15) finally yields

$$\sum_{n=-N}^{N} b_1(n)^2 = -k_1^2 + \frac{1}{k_1^2} + \sum_{n=-N}^{N} b(n)^2 + 2 \sum_{n=-N}^{N} \big(a(n)^2 - a_1(n-1)^2 \big).$$

The summands in all three sums vanish if n is sufficiently large or small. In particular we can rewrite the equation as

$$\sum_{n\in\mathbb{Z}} b_1(n)^2 = -k_1^2 + \frac{1}{k_1^2} + \sum_{n\in\mathbb{Z}} b(n)^2 + 2 \sum_{n\in\mathbb{Z}} \big(a(n)^2 - a_1(n)^2 \big).$$

The off-diagonal entries $a_1(n)$ are linked to $a(n)$ via (2.13) and we observe that

$$\prod_{n=-N}^{N} a_1(n)^2 = \prod_{n=-N}^{N} \frac{\varphi(n)}{\varphi(n+1)} \prod_{n=-N+1}^{N+1} \frac{\varphi(n+1)}{\varphi(n)} \prod_{n=-N}^{N} a(n)a(n+1)$$
$$= \frac{\varphi(-N)}{\varphi(-N+1)} \frac{\varphi(N+2)}{\varphi(N+1)} \prod_{n=-N}^{N} a(n)a(n+1)\,.$$

Recalling (2.11) and that $a(n) = a_1(n) = -1$ for sufficiently large $|n|$, this shows that

$$\prod_{n\in\mathbb{Z}} a_1(n)^2 = \frac{1}{k_1^2} \prod_{n\in\mathbb{Z}} a(n)^2\,.$$

If $\lambda_2 < -2$ we can now repeat the above procedure for the operator W_1. Starting from the eigenfunction φ for the lowest eigenvalue λ_2 of W_1 we can construct a new operator W_2 with off-diagonal entries a_2 and with potential b_2, which are defined as in (2.13) and (2.14), respectively, where a_1 now takes the place of a and λ_2 takes the place of λ_1. The operator W_2 then has the eigenvalues $\lambda_3, \dots, \lambda_M$ and it holds that

$$\sum_{n\in\mathbb{Z}} b_2(n)^2 = -k_2^2 + \frac{1}{k_2^2} + \sum_{n\in\mathbb{Z}} b_1(n)^2 + 2\sum_{n\in\mathbb{Z}} \left(a_1(n)^2 - a_2(n)^2\right)$$

as well as

$$\prod_{n\in\mathbb{Z}} a_2(n)^2 = \frac{1}{k_2^2} \prod_{n\in\mathbb{Z}} a_1(n)^2\,.$$

We can proceed in this manner eliminating all the negative eigenvalues and thus prove the following proposition.

Proposition 2.3.1 *Let W be the Jacobi operator (2.1) with $a(n) = -1$ and $b(n) = 0$ if $|n|$ is sufficiently large. Let $\lambda_1 < \dots < \lambda_L < -2$ be the negative eigenvalues of W and define $k_j > 1$ such that $\lambda_j = -k_j - \frac{1}{k_j}$. It holds that*

$$\sum_{n\in\mathbb{Z}} b_L(n)^2 = -\sum_{j=1}^{L} \left(k_j^2 - \frac{1}{k_j^2}\right) + \sum_{n\in\mathbb{Z}} b(n)^2 + 2\sum_{n\in\mathbb{Z}} \left(a(n)^2 - a_L(n)^2\right) \tag{2.18}$$

where the off-diagonal entries $a_L(n)$ and the potential $b_L(n)$ are obtained recursively by

the process described in detail above. It also holds that

$$\prod_{n\in\mathbb{Z}} a_L(n)^2 = \prod_{j=1}^{L} \frac{1}{k_j^2} \prod_{n\in\mathbb{Z}} a(n)^2 \,. \tag{2.19}$$

The Jacobi operator $(W_L u)(n) = a_L(n-1)u(n-1) + a_L(n)u(n+1) + b_L(n)u(n)$ has only positive eigenvalues $2 < \lambda_{L+1} < \cdots < \lambda_M$ and the property that $a_L(n) = -1$ and $b_L(n) = 0$ if $|n|$ is sufficiently large.

2.3.2 Elimination of Positive Eigenvalues

To eliminate the positive eigenvalues we have to proceed in a slightly different manner. The reason is that $W_L - \lambda_{L+1}$ is not a positive operator. This means that φ, the eigenfunction corresponding to λ_{L+1}, is not strictly positive, which can also be seen from the fact that $k_{L+1} < -1$ and that $\varphi(n) = ck_{L+1}^n$ for sufficiently small n. To circumvent this problem, we consider the new operator W_L', which is defined as

$$(W_L' u)(n) = a_L(n-1)u(n-1) + a_L(n)u(n+1) - b_L(n)u(n) \,.$$

If $\psi \in \ell^2(\mathbb{Z})$ is an eigenfunction of W_L with eigenvalue λ then $\psi'(n) = (-1)^n\psi(n)$ is also a sequence in $\ell^2(\mathbb{Z})$ and we compute that

$$(W_L'\psi')(n) = -(-1)^n(W_L\psi)(n) = -\lambda\psi'(n) \,.$$

Thus $-\lambda$ is an eigenvalue of W_L' and a similar computation shows that every eigenvalue η of W_L' corresponds to an eigenvalue $\lambda = -\eta$ of the operator W_L. We conclude that the eigenvalues of W_L' are exactly $-\lambda_M < \cdots < -\lambda_{L+1} < -2$. These eigenvalues can be written as $\eta_j = -\lambda_j = -\ell_j - \frac{1}{\ell_j}$ with $\ell_j = -k_j > 1$. The results of Proposition 2.3.1 now also hold for the operator W_L' and we thus obtain the identity

$$\sum_{n\in\mathbb{Z}} b_M(n)^2 = -\sum_{j=L+1}^{M} \left(\ell_j^2 - \frac{1}{\ell_j^2}\right) + \sum_{n\in\mathbb{Z}} b_L(n)^2 + 2\sum_{n\in\mathbb{Z}} \left(a_L(n)^2 - a_M(n)^2\right) \tag{2.20}$$

as well as

$$\prod_{n\in\mathbb{Z}} a_M(n)^2 = \prod_{j=L+1}^{M} \frac{1}{\ell_j^2} \prod_{n\in\mathbb{Z}} a_L(n)^2 \,. \tag{2.21}$$

The Jacobi operator W_M with potential b_M and off-diagonal entries a_M emerges from the (all-together) M-th elimination process in which we remove the last remaining eigenvalue $\eta_{L+1} = -\lambda_{L+1}$ from the spectrum and W_M has thus no eigenvalues outside of $[-2,2]$. Recalling that $\ell_j = -k_j$ we can combine (2.20) and (2.21) with (2.18) and (2.19) to obtain

$$\sum_{n\in\mathbb{Z}} b_M(n)^2 = -\sum_{j=1}^{M} \left(k_j^2 - \frac{1}{k_j^2}\right) + \sum_{n\in\mathbb{Z}} b(n)^2 + 2\sum_{n\in\mathbb{Z}} \left(a(n)^2 - a_M(n)^2\right) \tag{2.22}$$

and also

$$\prod_{n\in\mathbb{Z}} a_M(n)^2 = \prod_{j=1}^{M} \frac{1}{k_j^2} \prod_{n\in\mathbb{Z}} a(n)^2 \,. \tag{2.23}$$

The left-hand side of (2.22) is clearly positive, so we can deduce the inequality

$$\sum_{j=1}^{M} \left(k_j^2 - \frac{1}{k_j^2}\right) \leq \sum_{n\in\mathbb{Z}} b(n)^2 + 2\sum_{n\in\mathbb{Z}} (a(n)^2 - a_M(n)^2) \,. \tag{2.24}$$

We now aim to find an upper bound on the term $\sum_{n\in\mathbb{Z}} \left(a(n)^2 - a_M(n)^2\right)$ that only explicitly depends on $a(n)$ and the eigenvalues of W. To this end we apply the logarithmic function to both sides of (2.23) and derive

$$\sum_{n\in\mathbb{Z}} \left(\log a(n)^2 - \log a_M(n)^2\right) = \sum_{j=1}^{M} \log |k_j|^2 \,.$$

For positive real numbers $x \in (0,\infty)$ we have $\log x \leq x - 1$ and using this inequality and the identity above we can conclude that

$$\sum_{n\in\mathbb{Z}} \left(a(n)^2 - a_M(n)^2\right) \leq \sum_{j=1}^{M} \log |k_j|^2 + \sum_{n\in\mathbb{Z}} \left(a(n)^2 - 1 - \log a(n)^2\right) \,.$$

Inserting this inequality into (2.24) yields the desired result

$$\sum_{j=1}^{M}\left(k_j^2-\frac{1}{k_j^2}-\log|k_j|^4\right)\leq\sum_{n\in\mathbb{Z}}b(n)^2+2\sum_{n\in\mathbb{Z}}\left(a(n)^2-1-\log a(n)^2\right)\,.$$

It remains to extend this result to Jacobi operators which do not necessarily satisfy that $b(n)=0$ and $a(n)=-1$ for sufficiently large $|n|$. For a given Jacobi operator W and $N\in\mathbb{N}\cup\{0\}$ we define the truncation W_N as the Jacobi operator with potential and off-diagonal terms specified by

$$b_N(n)=\begin{cases}b(n), & |n|<N\\ 0, & |n|\geq N\,,\end{cases}\qquad\qquad a_N(n)=\begin{cases}a(n), & |n|<N\\ -1, & |n|\geq N\,.\end{cases}$$

In particular, for $N=0$ we obtain the free discrete Schrödinger operator $W_0=W_{-1,0}$ with $a_0(n)=-1$ and $b_0(n)=0$ for all $n\in\mathbb{Z}$. Each W_N fulfils the initial assumptions of our proof and thus satisfies inequality (2.6). If W is such that the right-hand side of (2.6) is finite, then $W-W_0$ is compact and a perturbation argument (see e.g. [44, Theorem 6.2]) shows that the left-hand side of (2.6) for W_N converges to the left-hand side of (2.6) for W as $N\to\infty$. Similarly the right-hand sides converge and thus the inequality also holds for W.

2.4 Proof of Theorem 2.2.2

For now we assume that the potential B vanishes if $|n|>n_{\max}$ and that also $A(n)=-\mathbb{I}$ for $|n|>n_{\max}$. These assumptions will later be dropped by a continuity argument but for the moment they guarantee that W has only finitely many eigenvalues outside of $[-2,2]$. Let these eigenvalues be denoted by

$$\lambda_1<\cdots<\lambda_L<-2<2<\lambda_{L+1}<\cdots<\lambda_M\,.$$

Each eigenvalue can be written as $\lambda_j=-k_j-\frac{1}{k_j}$ with $|k_j|\geq 1$ and has a multiplicity $m_j\leq m$. We assume that $\lambda_1<-2$ and thus $k_1>1$. Define Φ to be the matrix-solution of the equation

$$A(n-1)^*\Phi(n-1)+A(n)\Phi(n+1)+B(n)\Phi(n)=\lambda_1\Phi(n)$$

which satisfies

$$\Phi(n) = k_1^n \mathbb{I} \tag{2.25}$$

for $n < -n_{\max}$. Note that the quadratic form of W is given by

$$\langle Wu, u\rangle_{\ell^2} = \sum_{n\in\mathbb{Z}} \langle A(n-1)^* u(n-1) + A(n)u(n+1) + B(n)u(n), u(n)\rangle_{\mathbb{C}^m} \ . \tag{2.26}$$

Lemma 2.4.1 *$\Phi(n)$ is invertible for all $n \in \mathbb{Z}$. Furthermore $F(n) := -A(n)\Phi(n+1)\Phi(n)^{-1}$ is an invertible, Hermitian, positive-semidefinite matrix for all $n \in \mathbb{Z}$.*

Proof The proof of invertibility is adapted from a similar result [5] for the case of a Schrödinger operator on $L^2(\mathbb{R}, \mathbb{C}^m)$. The matrix function $\Phi(n)$ is by construction invertible for all $n < -n_{\max}$. Assume that there exists an $N \in \mathbb{N}$ and a $u \in \mathbb{C}^m$ such that $\Phi(N)u = 0$. Clearly the vector function $\Phi(n)u$ satisfies $(W - \lambda_1)\Phi(n)u = 0$. We can now define a new vector function φ as

$$\varphi(n) = \begin{cases} \Phi(n)u, & n < N \\ 0, & n \geq N \end{cases}$$

and from (2.26) we see that $\langle W\varphi, \varphi\rangle_{\ell^2} = \lambda_1 \langle \varphi, \varphi\rangle_{\ell^2}$. As λ_1 is the ground state we conclude that φ must therefore satisfy $(W - \lambda_1)\varphi = 0$. However, this implies that $\varphi(n) = 0$ for all $n \in \mathbb{N}$, which is a contradiction as $\Phi(n)$ is invertible for $n < -n_{\max}$.

We proceed in a similar way to the scalar case in [35] and note that $(W - \lambda_1) \geq 0$. For any $N \in \mathbb{Z}$ consider now the operator W_N which is defined as W restricted to the space $\ell^2(\mathbb{Z} \cap (-\infty, N), \mathbb{C}^m)$ with a Dirichlet boundary condition at N, i.e.

$$(W_N u)(n) = \begin{cases} (Wu)(n), & n \leq N-2 \\ A(N-2)^* u(n-2) + B(N-1)u(N-1), & n = N-1\,. \end{cases}$$

Then it holds that $(W_N - \lambda_1) \geq 0$. This can be proved by using the Min–Max principle to show that the lowest eigenvalue of W_N is larger than λ_1. Alternatively, we can write $W_N = P_N W P_N^*$ with projections P_N, P_N^* that cut off the matrix W below and to the right of the entry $B(N-1)$ such that $W_N - \lambda_1 = P_N(W - \lambda_1)P_N^* \geq 0$. Let $v \in \mathbb{C}^m$ be an arbitrary vector and consider the vector function $\varphi(n) = \Phi(n)\Phi(N)^{-1}A(N-1)^{-1}v$. By construction

it holds that $(W-\lambda_1)\varphi = 0$. We define the vector function $\psi \in \ell^2(\mathbb{Z}\cap(-\infty,N),\mathbb{C}^m)$ as $\psi(n)=\varphi(n)$ for $n \leq N-1$. For $n \leq N-2$ it holds that $\big((W_N-\lambda_1)\psi\big)(n)=0$ and for $n=N-1$ we calculate

$$\begin{aligned}\big((W_N-\lambda_1)\psi\big)(N-1) &= A(N-2)^*\psi(N-2)+\big(B(N-1)-\lambda_1\big)\psi(N-1)\\ &= -A(N-1)\varphi(N)\\ &= -v\end{aligned}$$

and thus conclude that $(W_N-\lambda_1)\psi = -\delta_{N-1}v$. Here δ_{N-1} is the operator that maps a vector $w\in\mathbb{C}^m$ onto the sequence $\delta_{N-1}w \in \ell^2(\mathbb{Z}\cap(-\infty,N),\mathbb{C}^m)$ whose entries are all zero except for $(\delta_{N-1}w)(N-1)=w$. As $(W_N-\lambda_1)\geq 0$ it holds that

$$\begin{aligned}0 \leq \langle (W_N-\lambda_1)\psi,\psi\rangle_{\ell^2} &= -\langle \delta_{N-1}v,\psi\rangle_{\ell^2} = -\langle v,\psi(N-1)\rangle_{\mathbb{C}^m}\\ &= -\big\langle v,\Phi(N-1)\Phi(N)^{-1}A(N-1)^{-1}v\big\rangle_{\mathbb{C}^m}\end{aligned}$$

This shows that $-A(N-1)\Phi(N)\Phi(N-1)^{-1}$ is a positive-semidefinite matrix and in particular Hermitian. □

Since $(W-\lambda_1)\Phi=0$, we can conclude that

$$A(n-1)^*\Phi(n-1)\Phi(n)^{-1}+A(n)\Phi(n+1)\Phi(n)^{-1}=\lambda_1-B(n)\,.$$

Using $F(n)=-A(n)\Phi(n+1)\Phi(n)^{-1}$, this can be written as a discrete Riccati-type equation

$$A(n-1)^*F(n-1)^{-1}A(n-1)+F(n)=B(n)-\lambda_1\,. \tag{2.27}$$

We now introduce the operator D on $\ell^2(\mathbb{Z},\mathbb{C}^m)$ as

$$(Du)(n)=F(n)^{-\frac{1}{2}}A(n)u(n+1)+F(n)^{\frac{1}{2}}u(n)\,,$$

where we note that by Lemma 2.4.1 the matrices $F(n)^{\pm 1/2}$ are well-defined. The adjoint of D is given by

$$(D^*u)(n)=A(n-1)^*F(n-1)^{-\frac{1}{2}}u(n-1)+F(n)^{\frac{1}{2}}u(n)\,.$$

Using (2.27) it can be shown that $D^*D = W - \lambda_1$. This identity allows us to conclude that the spectrum of the operator D^*D coincides with the spectrum of W, shifted by $-\lambda_1$. In particular, the eigenvalues of D^*D are $0, \lambda_2 - \lambda_1, \dots, \lambda_M - \lambda_1$ with multiplicities $m_1, \dots, m_M$. We also consider the operator DD^*, which can be written as $DD^* = W_1 - \lambda_1$, where W_1 is the Jacobi operator given by

$$(W_1 u)(n) = A_1(n-1)^* u(n-1) + A_1(n) u(n+1) + B_1(n) u(n)\,,$$

with off-diagonal entries

$$A_1(n) = F(n)^{-\frac{1}{2}} A(n) F(n+1)^{\frac{1}{2}} \tag{2.28}$$

and potential

$$B_1(n) = F(n)^{-\frac{1}{2}} A(n) A(n)^* F(n)^{-\frac{1}{2}} + F(n) + \lambda_1\,. \tag{2.29}$$

Note that $A_1(n) = -\mathbb{I}$ and $B_1(n) = 0$ if n is sufficiently small. A general result (see e.g. [19]) shows that with the possible exception of the eigenvalue zero, the operators D^*D and DD^* have the same eigenvalues with the same multiplicities. Assume that there is a non-vanishing function ψ such that $DD^*\psi = 0$. It follows that $D^*\psi = 0$ and as a consequence, for $n < -n_{\max}$, it must hold that

$$-\sqrt{\frac{1}{k_1}}\psi(n-1) + \sqrt{k_1}\psi(n) = 0\,.$$

Multiplying this equation by $\sqrt{k_1}$ we find that $\psi(n) = k_1^{-n} v$ with $v \in \mathbb{C}^m$. This function is clearly only in $\ell^2(-\mathbb{N}, \mathbb{C}^m)$ if $v = 0$, which implies that ψ vanishes everywhere. Consequently zero is not an eigenvalue of DD^*. Thus the Jacobi operator W_1 has precisely the eigenvalues $\lambda_2, \dots, \lambda_M$ with multiplicities $m_2, \dots, m_M$.

From the construction of F it immediately follows that $F(n) = k_1 \mathbb{I}$ for $n < -n_{\max}$ and thus

$$\operatorname{tr}\big(F(n)^{-1}\big) = m\frac{1}{k_1} \tag{2.30}$$

as well as

$$\operatorname{tr}\big(F(n)^{-2}\big) = m\frac{1}{k_1^2}\,. \tag{2.31}$$

The next result describes the behaviour of these terms if $n \to \infty$.

Lemma 2.4.2 *At any point $n_0 > n_{\max}$ the eigenvectors of $F(n_0)$ do not depend on n_0. The matrix $F(n_0)$ has an eigenvalue $\frac{1}{k_1}$ of multiplicity m_1 and every other eigenvalue $\mu(n_0)$ of $F(n_0)$ gives rise to a branch of eigenvalues $\mu(n)$ of $F(n)$ where $\mu(n)$ converges exponentially to k_1 for $n \to \infty$. In particular it holds that*

$$\lim_{n\to\infty} \operatorname{tr}\big(F(n)^{-1}\big) = m_1 k_1 + (m - m_1)\frac{1}{k_1} \tag{2.32}$$

as well as

$$\lim_{n\to\infty} \operatorname{tr}\big(F(n)^{-2}\big) = m_1 k_1^2 + (m - m_1)\frac{1}{k_1^2} \tag{2.33}$$

where the limits are achieved exponentially. Furthermore the potential $B_1(n)$ converges to 0 and the off-diagonal entries $A_1(n)$ converge to $-\mathbb{I}$ exponentially for $n \to \infty$.

Proof If $n > n_0 > n_{\max}$ then $\Phi(n) = Pk_1^{n-n_0} + Qk_1^{n_0-n}$ with matrices $P, Q \in \mathbb{C}^{m\times m}$. Since $(W - \lambda_1)\Phi = 0$ it must hold that

$$\begin{aligned} -\Phi(n_0) - \Phi(n_0+2) &= \lambda_1\Phi(n_0+1)\,,\\ -\Phi(n_0+1) - \Phi(n_0+3) &= \lambda_1\Phi(n_0+2)\,, \end{aligned}$$

and inserting $\Phi(n) = Pk_1^{n-n_0} + Qk_1^{n_0-n}$ into these two equations allows us to compute the matrices P and Q as

$$\begin{aligned} P &= \frac{k_1}{k_1^2-1}\left(-\frac{1}{k_1}\Phi(n_0) + \Phi(n_0+1)\right),\\ Q &= \frac{k_1}{k_1^2-1}\big(k_1\Phi(n_0) - \Phi(n_0+1)\big). \end{aligned}$$

Thus we can conclude that

$$\Phi(n) = \frac{k_1}{k_1^2-1}\left(\left(k_1^{n_0-n+1} - k_1^{n-n_0-1}\right)\Phi(n_0) + \left(k_1^{n-n_0} - k_1^{n_0-n}\right)\Phi(n_0+1)\right)$$

and as a consequence

$$\Phi(n) = \frac{k_1}{k_1^2 - 1} \left(k_1^{n_0 - n + 1} - k_1^{n - n_0 - 1} + \left(k_1^{n - n_0} - k_1^{n_0 - n} \right) F(n_0) \right) \Phi(n_0) \,. \tag{2.34}$$

Every eigenfunction φ of W to the eigenvalue λ_1 can be written as $\varphi(n) = \Phi(n)u$ with $u \in \mathbb{C}^m$. In order for φ to be square-summable, the parts in (2.34) that grow exponentially must vanish. As a consequence it must hold that $\varphi(n) = \Phi(n)\Phi(n_0)^{-1}v$ with $v \in \mathbb{C}^m$ such that $F(n_0)v = \frac{1}{k_1}v$. Since λ_1 is an m_1-fold eigenvalue of W we conclude that $F(n_0)$ has an m_1-fold eigenvalue $\frac{1}{k_1}$. From (2.34) we also conclude that $F(n) = f_n\big(F(n_0)\big)$ where

$$f_n(z) = \frac{k_1^{2n_0 - 2n} - 1 + \left(k_1 - k_1^{2n_0 - 2n - 1} \right) z}{k_1^{2n_0 - 2n + 1} - \frac{1}{k_1} + \left(1 - k_1^{2n_0 - 2n} \right) z} \,.$$

This shows that the eigenvectors of $F(n)$ are independent of n and that every eigenvalue μ of $F(n_0)$ generates an eigenvalue $\mu(n) = f_n(\mu)$ for $F(n)$. We see that $f_n\Big(\frac{1}{k_1}\Big) = \frac{1}{k_1}$ and $\lim_{n\to\infty} f_n(\mu) = k_1$ for all other eigenvalues μ.

As the eigenvectors of $F(n)$ do not depend on n, we can find a transformation T independent of n such that $F(n) = TE(n)T^{-1}$. The matrix $E(n)$ is diagonal with the first m_1 entries being $\frac{1}{k_1}$ followed by the other eigenvalues of $F(n)$. Using the definition (2.29) we see that $B_1(n) = T(E(n)^{-1} + E(n) + \lambda_1)T^{-1}$, which converges to 0 for $n \to \infty$ by the results above and the definition of k_1. Similarly it follows that $\lim_{n\to\infty} A(n) = -\lim_{n\to\infty} TE(n)^{-\frac{1}{2}}E(n+1)^{\frac{1}{2}}T^{-1} = -\mathbb{I}$. This completes the proof. □

We now aim to express $\sum_{n\in\mathbb{Z}} \operatorname{tr}\big(B_1(n)^2\big)$ in terms of k_1 and the potential B. To this end we recall (2.29) and compute that

$$\begin{aligned} \sum_{n\in\mathbb{Z}} \operatorname{tr}\big(B_1(n)^2\big) = \sum_{n\in\mathbb{Z}} \Bigg(& \operatorname{tr}\left(\left(F(n)^{-\frac{1}{2}} A(n) A(n)^* F(n)^{-\frac{1}{2}} + F(n) \right)^2 \right) \\ & + 2\lambda_1 \operatorname{tr}\left(F(n)^{-\frac{1}{2}} A(n) A(n)^* F(n)^{-\frac{1}{2}} + F(n) \right) + m\lambda_1^2 \Bigg). \end{aligned} \tag{2.35}$$

Using (2.27) and the cyclicity of the trace we can deduce that for any natural number N the identity

$$\begin{aligned}
&\sum_{n=-N}^{N} \operatorname{tr}\left(F(n)^{-\frac{1}{2}}A(n)A(n)^*F(n)^{-\frac{1}{2}} + F(n)\right) \\
&= \sum_{n=-N+1}^{N+1} \operatorname{tr}\big(A(n-1)^*F(n-1)^{-1}A(n-1)\big) + \sum_{n=-N}^{N} \operatorname{tr}\big(F(n)\big) \\
&= \operatorname{tr}\big(A(N)^*F(N)^{-1}A(N)\big) - \operatorname{tr}\big(A(-N-1)^*F(-N-1)^{-1}A(-N-1)\big) \\
&\quad + \sum_{n=-N}^{N} \operatorname{tr}\big(B(n)-\lambda_1\big)
\end{aligned}$$

holds. We can compute the two terms outside the sum by choosing N sufficiently large such that $A(N) = A(N-1) = -\mathbb{I}$. From (2.30) we then obtain

$$\begin{aligned}
\sum_{n=-N}^{N} \operatorname{tr}\left(F(n)^{-\frac{1}{2}}A(n)A(n)^*F(n)^{-\frac{1}{2}} + F(n)\right) &= \operatorname{tr}\big(F(N)^{-1}\big) - m\frac{1}{k_1} \\
&\quad + \sum_{n=-N}^{N} \operatorname{tr}\big(B(n)-\lambda_1\big).
\end{aligned} \tag{2.36}$$

It remains to treat the quadratic terms in (2.35) and to this end we consider the square of equation (2.27). This, together with the cyclicity of the trace, enables us to conclude that

$$\begin{aligned}
&\sum_{n=-N}^{N} \operatorname{tr}\left(\left(F(n)^{-\frac{1}{2}}A(n)A(n)^*F(n)^{-\frac{1}{2}} + F(n)\right)^2\right) \\
&= \sum_{n=-N}^{N} \left(\operatorname{tr}\left(\left(A(n)^*F(n)^{-1}A(n)\right)^2\right) + 2\operatorname{tr}\big(A(n)A(n)^*\big) + \operatorname{tr}\left(F(n)^2\right)\right) \\
&= \sum_{n=-N+1}^{N+1} \operatorname{tr}\left(\left(A(n-1)^*F(n-1)^{-1}A(n-1)\right)^2\right) + \sum_{n=-N}^{N} \operatorname{tr}\left(F(n)^2 + 2A(n)A(n)^*\right) \\
&= \operatorname{tr}\left(\left(A(N)^*F(N)^{-1}A(N)\right)^2\right) - \operatorname{tr}\left(\left(A(-N-1)^*F(-N-1)^{-1}A(-N-1)\right)^2\right) \\
&\quad + \sum_{n=-N}^{N} \operatorname{tr}\left(\left(B(n)-\lambda_1\right)^2 - 2A(n-1)^*F(n-1)^{-1}A(n-1)F(n) + 2A(n)A(n)^*\right).
\end{aligned}$$

Using once again that for N sufficiently large $A(N) = A(-N-1) = -\mathbb{I}$, and recalling (2.28) as well as (2.31), we arrive at

$$\sum_{n=-N}^{N} \operatorname{tr}\left(\left(F(n)^{-\frac{1}{2}}A(n)A(n)^*F(n)^{-\frac{1}{2}} + F(n)\right)^2\right) = \operatorname{tr}\big(F(N)^{-2}\big) - m\frac{1}{k_1^2} + \sum_{n=-N}^{N} \operatorname{tr}\left(\big(B(n)-\lambda_1\big)^2 - 2A_1(n-1)A_1(n-1)^* + 2A(n)A(n)^*\right).$$

Combining this with (2.35) and (2.36) we obtain the identity

$$\sum_{n=-N}^{N} \operatorname{tr}\big(B_1(n)^2\big) = \operatorname{tr}\big(F(N)^{-2}\big) - m\frac{1}{k_1^2} + 2\lambda_1\left(\operatorname{tr}\big(F(N)^{-1}\big) - m\frac{1}{k_1}\right) + \sum_{n=-N}^{N} \operatorname{tr}\big(B(n)^2\big) + 2\sum_{n=-N}^{N} \operatorname{tr}\big(A(n)A(n)^* - A_1(n-1)A_1(n-1)^*\big).$$

Recalling (2.32) and (2.33) as well as $\lambda_1 = -k_1 - \frac{1}{k_1}$ yields

$$\lim_{N\to\infty}\left(\operatorname{tr}\big(F(N)^{-2}\big) - m\frac{1}{k_1^2} + 2\lambda_1\left(\operatorname{tr}\big(F(N)^{-1}\big) - m\frac{1}{k_1}\right)\right) = m_1\frac{1}{k_1^2} - m_1k_1^2$$

and consequently we finally arrive at

$$\sum_{n\in\mathbb{Z}} \operatorname{tr}\big(B_1(n)^2\big) = m_1\frac{1}{k_1^2} - m_1k_1^2 + \sum_{n\in\mathbb{Z}} \operatorname{tr}\big(B(n)^2\big) + 2\sum_{n\in\mathbb{Z}} \operatorname{tr}\big(A(n)A(n)^* - A_1(n-1)A_1(n-1)^*\big).$$

Since $\lim_{|n|\to\infty} A_1(n) = -\mathbb{I}$, we can replace $A_1(n-1)A_1(n-1)^*$ in the above identity by $A_1(n)A_1(n)^*$. The off-diagonal entries $A_1(n)$ are linked to $A(n)$ via (2.28). Thus we can

compute that

$$\begin{aligned}
&\sum_{n=-N}^{N} \log\det\big(A_1(n)A_1(n)^*\big) \\
&= \sum_{n=-N}^{N} \log\det(A(n)F(n+1)A(n)^*F(n)^{-1}\big) \\
&= \sum_{n=-N}^{N} \big(\log\det F(n+1) - \log\det F(n) + \log\det\big(A(n)A(n)^*\big)\big) \\
&= \log\det F(N+1) - \log\det F(-N) + \sum_{n=-N}^{N} \log\det\big(A(n)A(n)^*\big).
\end{aligned}$$

Letting $N \to \infty$ we obtain from (2.25) and Lemma 2.4.2 that

$$\sum_{n\in\mathbb{Z}} \log\det\big(A_1(n)A_1(n)^*\big) = -m_1 \log|k_1|^2 + \sum_{n\in\mathbb{Z}} \log\det\big(A(n)A(n)^*\big).$$

We summarise our results in the following proposition.

Proposition 2.4.3 *Let W be the Jacobi operator (2.7) with $B(n) = 0$ and $A(n) = -\mathbb{I}$ for sufficiently large $|n|$. Let $\lambda_1 < \cdots < \lambda_L < -2 < 2 < \lambda_{L+1} < \cdots < \lambda_M$ be the eigenvalues of W each with multiplicity $m_j \le m$ and define $|k_j| > 1$ such that $\lambda_j = -k_j - \frac{1}{k_j}$. Then it holds that*

$$\begin{aligned}
\sum_{j=1}^{M} m_j \left(\frac{1}{k_j^2} - k_j^2 + \log|k_j|^4\right) - m_1 \log|k_1|^4 + \sum_{n\in\mathbb{Z}} \operatorname{tr}\big(B(n)^2\big) \\
+ 2\sum_{n\in\mathbb{Z}} \operatorname{tr}\big(A(n)A(n)^* - A_1(n)A_1(n)^*\big) \\
= \sum_{j=2}^{M} m_j \left(\frac{1}{k_j^2} - k_j^2 + \log|k_j|^4\right) + \sum_{n\in\mathbb{Z}} \operatorname{tr}\big(B_1(n)^2\big)
\end{aligned}$$

where the off-diagonal entries $A_1(n)$ and the potential $B_1(n)$ are defined as in (2.28) and (2.29), respectively. It also holds that

$$\sum_{n\in\mathbb{Z}} \log\det\big(A_1(n)A_1(n)^*\big) = -m_1 \log|k_1|^2 + \sum_{n\in\mathbb{Z}} \log\det\big(A(n)A(n)^*\big).$$

Unfortunately we cannot repeat this procedure immediately. While (2.25) implies that $B_1(n) = 0$ and $A_1(n) = -\mathbb{I}$ for sufficiently small n, it only holds that $B_1(n)$ decays exponentially fast for $n \to \infty$. Thus the potential does not necessarily vanish for sufficiently large n. Similarly $A_1(n)$ converges exponentially fast to $-\mathbb{I}$ as $n \to \infty$ but $A_1(n) = -\mathbb{I}$ may not hold for sufficiently large n. Thus we have to introduce a cut after which we set $A_1(n)$ to be $-\mathbb{I}$ and $B_1(n)$ to be zero. With fixed $N^c > n_{\max}$ let the operator W_1^c be defined as

$$(W_1^c u)(n) = A_1^c(n-1)^* u(n-1) + A_1^c(n) u(n+1) + B_1^c(n) u(n)$$

where

$$A_1^c(n) = \begin{cases} A_1(n) & , n < N^c \\ -\mathbb{I} & , n \geq N^c, \end{cases} \qquad B_1^c(n) = \begin{cases} B_1(n) & , n < N^c \\ 0 & , n \geq N^c. \end{cases}$$

The new Jacobi operator W_1^c satisfies all the conditions of Proposition 2.4.3. It has eigenvalues $\mu_j = -\ell_j^2 - \frac{1}{\ell_j^2}$ with $|\ell_j| > 1$ for $j \in \{2, \dots, M^c\}$ and corresponding multiplicities n_j which are not necessarily the same as the eigenvalues and multiplicities of W_1. However, the first $m_2 + \cdots + m_M$ eigenvalues (counted with multiplicity), say $\mu_2, \dots, \mu_{M'}$ with $n_2 + \cdots + n_{M'} = m_2 + \cdots + m_M$, can be made arbitrarily close to the original eigenvalues $\lambda_2, \dots, \lambda_M$ (counted with multiplicity) by choosing N^c sufficiently large. The potential additional eigenvalues $\mu_{M'+1}, \dots, \mu_{M^c}$ can be made as close to the essential spectrum as we please. Proposition 2.4.3 now implies that

$$\begin{aligned} \sum_{j=2}^{M^c} n_j \left(\frac{1}{\ell_j^2} - \ell_j^2 + \log |\ell_j|^4 \right) - n_2 \log |\ell_2|^4 + \sum_{n \in \mathbb{Z}} \operatorname{tr}\big(B_1^c(n)^2\big) \\ + 2 \sum_{n \in \mathbb{Z}} \operatorname{tr}\big(A_1^c(n) A_1^c(n)^* - A_2(n) A_2(n)^*\big) \\ = \sum_{j=3}^{M^c} n_j \left(\frac{1}{\ell_j^2} - \ell_j^2 + \log |\ell_j|^4 \right) + \sum_{n \in \mathbb{Z}} \operatorname{tr}\big(B_2(n)^2\big) \end{aligned}$$

and also

$$\sum_{n \in \mathbb{Z}} \log \det \left(A_2(n) A_2(n)^* \right) = -n_2 \log |\ell_1|^2 + \sum_{n \in \mathbb{Z}} \log \det \left(A_1^c(n) A_1^c(n)^* \right).$$

As a consequence we obtain that

$$\begin{aligned}\sum_{j=1}^{M} m_j\left(\frac{1}{k_j^2}-k_j^2+\log|k_j|^4\right)-m_1\log|k_1|^4-n_2\log|\ell_2|^4+\sum_{n\in\mathbb{Z}}\operatorname{tr}\big(B(n)^2\big)\\ +2\sum_{n\in\mathbb{Z}}\operatorname{tr}\big(A(n)A(n)^*-A_2(n)A_2(n)^*\big)\\ =e_2+\sum_{j=3}^{M'} n_j\left(\frac{1}{\ell_j^2}-\ell_j^2+\log|\ell_j|^4\right)+\sum_{n\in\mathbb{Z}}\operatorname{tr}\big(B_2(n)^2\big)\end{aligned}$$

with an error e_2 stemming from the error in the eigenvalues and from substituting M' for M^c as well as from replacing the matrix functions B_1^c and A_1^c by B_1 and A_1, respectively. Note that the total number of eigenvalues (counted with multiplicities) over which we sum on the right-hand side is $m_2+\cdots+m_M-n_2$ and thus strictly smaller than $m_2+\cdots+m_M$. It also holds that

$$\begin{aligned}\sum_{n\in\mathbb{Z}}\log\det\big(A_2(n)A_2(n)^*\big)=&-m_1\log|k_1|^2-n_2\log|\ell_2|^2+f_2\\ &+\sum_{n\in\mathbb{Z}}\log\det\big(A(n)A(n)^*\big)\end{aligned}$$

with an error f_2 correcting the replacement of A_1^c by A_2. We can now introduce a cut in A_2 and B_2 and repeat the above steps to eliminate all the positive eigenvalues. For the negative eigenvalues we proceed as in the scalar case, using the unitary transformation $(Uu)(n)=(-1)^n u(n)$. After a finite number of $s\le m_1+\cdots+m_M$ steps, we arrive at

$$\begin{aligned}&\sum_{j=1}^{M} m_j\left(\frac{1}{k_j^2}-k_j^2+\log|k_j|^4\right)-m_1\log|k_1|^4-n_2\log|\ell_2|^4-\cdots-q_s\log|p_s|^4\\ &+\sum_{n\in\mathbb{Z}}\operatorname{tr}\big(B(n)^2\big)+2\sum_{n\in\mathbb{Z}}\operatorname{tr}\big(A(n)A(n)^*-A_s(n)A_s(n)^*\big)\\ &=e_2+\cdots+e_s+\sum_{n\in\mathbb{Z}}\operatorname{tr}\big(B_s(n)^2\big)\\ &\ge e_2+\cdots+e_s\end{aligned}\tag{2.37}$$

with

$$\sum_{n\in\mathbb{Z}} \log\det\big(A_s(n)A_s(n)^*\big) = -\,m_1\log|k_1|^2 - n_2\log|\ell_2|^2 - \cdots - q_s\log|p_s|^2 \\ + f_2 + \cdots + f_s + \sum_{n\in\mathbb{Z}} \log\det\big(A(n)A(n)^*\big). \tag{2.38}$$

Fix $n \in \mathbb{N}$ and note that $A_s(n)A_s(n)^*$ is Hermitian, positive semi-definite and invertible. Let $\mu_1, \ldots, \mu_m$ denote the eigenvalues of this matrix, which are necessarily real and positive. Then, using $\log x \leq x - 1$ for $x \in (0, \infty)$, we obtain that

$$\operatorname{tr}\big(\mathbb{I} - A_s(n)A_s(n)^*\big) = \sum_{j=1}^{m} 1 - \mu_j \leq -\sum_{j=1}^{m} \log\mu_j = -\log\det\big(A_s(n)A_s(n)^*\big).$$

This allows us to conclude from (2.37) and (2.38) that

$$\sum_{j=1}^{M} m_j\left(k_j^2 - \frac{1}{k_j^2} - \log|k_j|^4\right) + e_2 + \cdots + e_s + f_2 + \cdots + f_s \\ \leq \sum_{n\in\mathbb{Z}} \operatorname{tr}\big(B(n)^2\big) + 2\sum_{n\in\mathbb{Z}} \Big(\operatorname{tr}\big(A(n)A(n)^* - \mathbb{I}\big) - \log\det\big(A(n)A(n)^*\big)\Big)\,.$$

All the errors $e_2, \ldots, e_s$ and $f_2, \ldots, f_s$ can be made arbitrarily small such that we get the desired result (2.8). Using an approximation argument, this inequality extends to Jacobi operators W which only satisfy that the right-hand side of (2.8) is finite.

2.5 Proof of Theorem 2.2.3

Adapting the Aizenman–Lieb principle [2], we aim to prove spectral inequalities which depend on higher powers of the eigenvalues λ_j and the potential B. In this section we shall restrict ourselves to the case of a discrete Schrödinger operator such that $A(n) = -\mathbb{I}$ for all $n \in \mathbb{Z}$. Let λ_j^+ for $j = 1, \ldots, M^+$ denote the eigenvalues of W that are larger than 2 and let $1 \leq m_j^+ \leq m$ denote their respective multiplicities. In complete analogy we define λ_j^- for $j = 1, \ldots, M^-$ as the eigenvalues which are smaller than -2 and denote their multiplicities by m_j^-. In the following computations we will at times consider the positive/negative eigenvalues of a discrete Schrödinger operator W with potential B' different to B. Whenever we do so, we will denote these eigenvalues by $\lambda_j^\pm(B')$ to make a clear distinction.

Hundertmark and Simon [42] showed that the inequalities

$$\sum_{j=1}^{M^\pm} m_j^\pm \big((\lambda_j^\pm)^2 - 4\big)^{\frac{1}{2}} \leq \sum_{n\in\mathbb{Z}} \operatorname{tr}\big(B(n)_\pm\big) \tag{2.39}$$

hold. As noted in [68], a straightforward calculation shows that

$$\frac{1}{2}\left(k^2 - \frac{1}{k^2} - \log|k|^4\right) = \int_2^{|\lambda|} (E^2-4)^{\frac{1}{2}}\,\mathrm{d}E \tag{2.40}$$

for $-k - \frac{1}{k} = \lambda \in \mathbb{R}\setminus[-2,2]$ with $|k| > 1$. This raises the question of whether we can derive (2.9) from the result by Hundertmark and Simon (2.39) and whether we can then obtain similar inequalities for higher powers of the eigenvalues by considering iterated integrals of $(E^2-4)^{\frac{1}{2}}$. To this end, we compute that for $\gamma > \frac{1}{2}$

$$\begin{aligned}
&\sum_{j=1}^{M^+} m_j^+ \int_2^{\lambda_j^+} (E^2-4)^{\frac{1}{2}} (\lambda_j^+ - E)^{\gamma-\frac{3}{2}}\,\mathrm{d}E \\
&= \int_0^\infty \sum_{j=1}^{M^+} m_j^+ \big((\lambda_j^+ - t)^2 - 4\big)^{\frac{1}{2}} t^{\gamma-\frac{3}{2}} \chi_{\{\lambda_j^+ - t \geq 2\}}(t)\,\mathrm{d}t \\
&= \int_0^\infty \sum_{j=1}^{M^+} m_j^+ \big(\lambda_j^+ (B-t)^2 - 4\big)^{\frac{1}{2}} t^{\gamma-\frac{3}{2}} \chi_{\{\lambda_j^+(B-t) \geq 2\}}(t)\,\mathrm{d}t\,,
\end{aligned}$$

where we have used the substitution $t = \lambda_j^+ - E$. Note that by the Min–Max principle $\lambda_j^+(B-t) \leq \lambda_j^+\big((B-t)_+\big)$ and thus we obtain from (2.39) that

$$\sum_{j=1}^{M^+} m_j^+ \int_2^{\lambda_j^+} (E^2-4)^{\frac{1}{2}} (\lambda_j^+ - E)^{\gamma-\frac{3}{2}}\,\mathrm{d}E \leq \sum_{n\in\mathbb{Z}} \int_0^\infty t^{\gamma-\frac{3}{2}} \operatorname{tr}\big((B(n)-t)_+\big)\,\mathrm{d}t\,.$$

Let $\mu_1(n), \ldots, \mu_\ell(n)$ with $\ell(n) \leq m$ be the eigenvalues of $B(n)$ which are positive. We

observe that for fixed $n \in \mathbb{Z}$

$$\begin{aligned}\int_0^\infty t^{\gamma-\frac{3}{2}} \operatorname{tr}\big((B(n)-t)_+\big)\,\mathrm{d}t &= \sum_{k=1}^{\ell(n)} \int_0^\infty t^{\gamma-\frac{3}{2}} \big(\mu_k(n)-t\big)_+\,\mathrm{d}t \\ &= \sum_{k=1}^{\ell(n)} \mu_k(n)^{\gamma+\frac{1}{2}} \int_0^1 s^{\gamma-\frac{3}{2}}(1-s)\,\mathrm{d}s \\ &= \mathrm{B}\left(\gamma-\frac{1}{2},2\right) \operatorname{tr}\left(B(n)_+^{\gamma+\frac{1}{2}}\right)\end{aligned}$$

with the simplified notation $B(n)_+^{\gamma+1/2} = \big(B(n)_+\big)^{\gamma+1/2}$ and the Beta function $\mathrm{B}(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}$. As a consequence it holds that

$$\sum_{j=1}^{M^+} m_j^+ \int_2^{\lambda_j^+} (E^2-4)^{\frac{1}{2}} (\lambda_j^+ - E)^{\gamma-\frac{3}{2}}\,\mathrm{d}E \leq \mathrm{B}\left(\gamma-\frac{1}{2},2\right) \sum_{n\in\mathbb{Z}} \operatorname{tr}\left(B(n)_+^{\gamma+\frac{1}{2}}\right)$$

and in complete analogy it is possible to show that

$$\sum_{j=1}^{M^-} m_j^- \int_2^{|\lambda_j^-|} (E^2-4)^{\frac{1}{2}} (|\lambda_j^-| - E)^{\gamma-\frac{3}{2}}\,\mathrm{d}E \leq \mathrm{B}\left(\gamma-\frac{1}{2},2\right) \sum_{n\in\mathbb{Z}} \operatorname{tr}\left(B(n)_-^{\gamma+\frac{1}{2}}\right).$$

Together these two results prove the main result (2.10) of Theorem 2.2.3. Defining $|k_j| \geq 1$ via $\lambda_j = -k_j - \frac{1}{k_j}$, the inequality coincides for $\gamma = \frac{3}{2}$ by (2.40) with (2.9).

For half-integers values $\gamma \in \mathbb{N} + \frac{1}{2}$ the substitution $E = t + 1/t$ allows us to explicitly compute the left-hand side of (2.10) in terms of k_j and we observe the emergence of logarithmic terms of k_j. In these cases it is also possible to compute the left-hand side of the

inequality in terms of λ_j and for $\gamma = \frac{3}{2}, \frac{5}{2}$ we get

$$\sum_{j\geq 1} m_j \left(2\log 2 + \frac{1}{2}|\lambda_j|(\lambda_j^2-4)^{\frac{1}{2}} - 2\log\left(|\lambda_j| + (\lambda_j^2-4)^{\frac{1}{2}}\right)\right)$$
$$\leq \frac{1}{2}\sum_{n\in\mathbb{Z}} \operatorname{tr}\left(|B(n)|^2\right),$$
$$\sum_{j\geq 1} m_j \left(2|\lambda_j|\log 2 + \frac{1}{2}\lambda_j^2(\lambda_j^2-4)^{\frac{1}{2}} - 2|\lambda_j|\log\left(|\lambda_j| + (\lambda_j^2-4)^{\frac{1}{2}}\right) - \frac{1}{3}(\lambda_j^2-4)^{\frac{3}{2}}\right)$$
$$\leq \frac{1}{6}\sum_{n\in\mathbb{Z}} \operatorname{tr}\left(|B(n)|^3\right).$$

In the scalar case $m = 1$ we can use the same method as in [42] to pass from inequalities in the case $a \equiv -1$ to the general case where $a(n) \to -1$ as $|n| \to \infty$. This method was described in Section 2.1 and it yields the following result.

Theorem 2.5.1 *Let W be the scalar Jacobi operator (2.1) and enumerate the eigenvalues outside of $[-2,2]$ as $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq 2$. Then it holds for $\gamma > \frac{1}{2}$ that*

$$\sum_{j\geq 1} \int_2^{|\lambda_j|} (E^2-4)^{\frac{1}{2}}(|\lambda_j| - E)^{\gamma-\frac{3}{2}}\,\mathrm{d}E$$
$$\leq 3^{\gamma-\frac{1}{2}}\mathrm{B}\left(\gamma-\frac{1}{2},2\right)\left(\sum_{n\in\mathbb{Z}}|b(n)|^{\gamma+\frac{1}{2}} + 4\sum_{n\in\mathbb{Z}}|a(n)+1|^{\gamma+\frac{1}{2}}\right).$$

2.6 Sharpness of the Inequalities

In this section we will discuss whether the obtained inequalities are sharp and whether optimisers exist.

2.6.1 Inequalities of Theorem 2.2.1 and Theorem 2.2.2

We aim to show that inequality (2.6) is sharp. This clearly also implies that the more general inequality (2.8) is sharp for all $m \geq 1$ as we can simply consider diagonal matrix-functions A, B. In [70] (see also [69]) examples of reflectionless potentials for the Jacobi operator were constructed using Darboux transformations. The obtained operators are of the form

$$(\widetilde{W}u)(n) = \widetilde{a}(n+1)u(n+1) + u(n-1) + \widetilde{b}(n)u(n)$$

which can easily be transformed to the Hermitian form (2.1). Let $\omega > 0$ and define $c_n := \cosh(\omega n)$. The examples of Spiridonov and Zhedanov let us conclude that the Jacobi operator W_1 of the form (2.1) with potential

$$b_1(n) = \frac{c_n}{c_{n+1}} - \frac{c_{n-1}}{c_n}$$

and off-diagonal entries

$$a_1(n) = -\frac{\sqrt{c_n c_{n+2}}}{c_{n+1}}$$

is reflectionless and has one eigenvalue $\lambda_1 = -2\cosh(\omega) < -2$. Since $k_1 = \mathrm{e}^{\omega}$ we observe that

$$k_1^2 - \frac{1}{k_1^2} - \log|k_1|^4 = \mathrm{e}^{2\omega} - \mathrm{e}^{-2\omega} - 4\omega \tag{2.41}$$

and it remains to prove that the right-hand side of (2.6) converges to this value. Note that W_1 can also be obtained by applying the commutation method to the free discrete Schrödinger operator $W_0 = W_{-1,0}$ with $a \equiv -1$ and $b \equiv 0$. To this end we observe that $\varphi(n) = \cosh(\omega n) \notin \ell^2(\mathbb{Z})$ is a solution to the equation $W_0\varphi = \lambda_1\varphi$. As shown by Gesztesy and Teschl [35] in a general setting, the Jacobi operator with potential given by (2.14) and off-diagonal entries (2.13) now has exactly one eigenvalue λ_1. It is easy to check that this operator is precisely the operator W_1 since

$$b_1(n) = \frac{c_n}{c_{n+1}} - \frac{c_{n-1}}{c_n} = \frac{c_n}{c_{n+1}} + \frac{c_{n+1}}{c_n} + \lambda_1\,.$$

Note that the difference to our previous work is that here we start with a real number λ_1 which is no eigenvalue of W_0 and create an operator W_1 that has exactly one eigenvalue λ_1. In the previous sections we started with the ground state of a Jacobi operator and eliminated this point from the spectrum by means of exactly the same method.

Using (2.15) and repeating the calculations thereafter together with the facts that

$$\lim_{N\to\infty} \frac{c_N}{c_{N+1}} = \mathrm{e}^{-\omega}\,,\ \lim_{N\to\infty} \frac{c_{-N-1}}{c_{-N}} = \mathrm{e}^{\omega}\,,$$

we can show that

$$\sum_{n\in\mathbb{Z}} b_1(n)^2 = -\mathrm{e}^{-2\omega} + \mathrm{e}^{2\omega} + 2\sum_{n\in\mathbb{Z}}(1 - a_1(n)^2)\,. \tag{2.42}$$

It is easy to see that $\sum_{n\in\mathbb{Z}} \log a_1(n)^2$ is a telescoping series such that

$$\begin{aligned}\sum_{n=-N}^{N} \log a_1(n)^2 &= \sum_{n=-N}^{N}\left(\log\left(\frac{c_n}{c_{n+1}}\right) - \log\left(\frac{c_{n+1}}{c_{n+2}}\right)\right)\\ &= \log\left(\frac{c_{-N}}{c_{-N+1}}\right) - \log\left(\frac{c_{N+1}}{c_{N+2}}\right),\end{aligned}$$

which converges to 2ω as $N \to \infty$. Thus

$$2\sum_{n\in\mathbb{Z}} \log a_1(n)^2 = 4\omega$$

and together with (2.41) and (2.42) we can conclude that for this special reflectionless operator W_1 there is equality in (2.6).

Note that the Darboux transformations used by Spiridonov and Zhedanov do not allow one to construct a potential b for any given off-diagonal entries a such that the Jacobi operator becomes reflectionless. In particular, it is not possible to construct a reflectionless Jacobi operator with $a \equiv -1$.

However, in [70] a second example of a reflectionless Jacobi operator can be found which has vanishing potential $b \equiv 0$ and non-trivial off-diagonal entries. The operator W with $b \equiv 0$ and off-diagonal entries

$$a(n) = -\sqrt{\frac{c_{n-1}c_{n+2}}{c_n c_{n+1}}}$$

has the two eigenvalues $\lambda_1 = -2\cosh(\omega) < -2$ and $\lambda_2 = 2\cosh(\omega) > 2$. We observe that $k_1 = \mathrm{e}^{\omega}$ and $k_2 = -\mathrm{e}^{\omega}$ such that

$$\sum_{j=1}^{2}\left(k_j^2 - \frac{1}{k_j^2} - \log|k_j|^4\right) = 2\left(\mathrm{e}^{2\omega} - \mathrm{e}^{-2\omega} - 4\omega\right)\,. \tag{2.43}$$

It remains to prove that the series on the right-hand side of (2.6) converges to this value. Note that due to the symmetry properties of $\cosh x$ it holds that $a(n) = a(-n-1)$ and

consequently

$$\sum_{n\in\mathbb{Z}} \left(a(n)^2 - 1 - \log a(n)^2\right) = 2\sum_{n=0}^{\infty} \left(a(n)^2 - 1 - \log a(n)^2\right) \tag{2.44}$$

We first consider the series $\sum_{n=0}^{\infty} \log a(n)^2$ which can be proved to be a telescoping series such that

$$\sum_{n=0}^{N} \log a(n)^2 = \sum_{n=0}^{N} \left(\log\left(\frac{c_{n-1}}{c_n}\right) - \log\left(\frac{c_{n+1}}{c_{n+2}}\right)\right) = -\log\left(\frac{c_N}{c_{N+1}}\right) - \log\left(\frac{c_{N+1}}{c_{N+2}}\right).$$

It is easy to verify that $\lim_{N\to\infty} \log\left(\frac{c_N}{c_{N+1}}\right) = \lim_{N\to\infty} \log\left(\frac{c_{N+1}}{c_{N+2}}\right) = -\omega$ and as a consequence we obtain that

$$\sum_{n=0}^{\infty} \log a(n)^2 = 2\omega\,. \tag{2.45}$$

Similarly we can treat the series $\sum_{n=0}^{\infty} \left(a(n)^2 - 1\right)$ and a simple computation shows that

$$\begin{aligned}\sum_{n=0}^{N} \left(a(n)^2 - 1\right) &= \left(\mathrm{e}^{2\omega} - \mathrm{e}^{-2\omega}\right) \sum_{n=0}^{N} \left(\frac{1}{\mathrm{e}^{2n\omega}+1} - \frac{1}{\mathrm{e}^{(2n+2)\omega}+1}\right) \\ &= \left(\mathrm{e}^{2\omega} - \mathrm{e}^{-2\omega}\right) \left(\frac{1}{2} - \frac{1}{\mathrm{e}^{(2N+2)\omega}+1}\right).\end{aligned}$$

Letting $N \to \infty$ we observe that

$$\sum_{n=0}^{\infty} \left(a(n)^2 - 1\right) = \frac{\mathrm{e}^{2\omega} - \mathrm{e}^{-2\omega}}{2}\,. \tag{2.46}$$

Inserting (2.45) and (2.46) into (2.44) and recalling (2.43) we conclude that for the special choices of $a(n)$ and $b(n)$ the spectral inequality (2.6) is in fact an equality.

These results point out an important similarity between (2.6) and the Lieb–Thirring inequality on the continuum for the power $\gamma = \frac{3}{2}$. Both inequalities are sharp for reflectionless potentials. While we have given two explicit examples of reflectionless Jacobi operators and have shown by direct computation that these operators both yield an equality in (2.6), this statement is in fact true for any reflectionless Jacobi operator. In [44] inequality (2.6) was obtained from an identity that consists of an additional term involving the

transmission coefficient. From this identity it can be seen that (2.6) becomes an equality if and only if the Jacobi operator is reflectionless. The two explicit examples in this thesis were discussed to illustrate this equivalence and to emphasise the connection between the creation and the elimination of eigenvalues of Jacobi operators.

2.6.2 Inequalities of Theorem 2.2.3

We will now show some general properties of the left-hand side of (2.10). We are interested in its behaviour for large eigenvalues as well as for eigenvalues which are close to the essential spectrum. To this end we define the function $G_\gamma(\lambda)$ for $\lambda > 2$ and $\gamma > \frac{1}{2}$ as

$$G_\gamma(\lambda) = \int_2^\lambda (E^2-4)^{\frac{1}{2}}(\lambda - E)^{\gamma-\frac{3}{2}}\,\mathrm{d}E$$

which allows us write the left-hand side of (2.10) simply as $\sum_{j\geq 1} m_j G_\gamma(|\lambda_j|)$.

Lemma 2.6.1 *For $\lambda \to 2$ we observe the asymptotic behaviour*

$$G_\gamma(\lambda) = 2\mathrm{B}\left(\gamma - \frac{1}{2}, \frac{3}{2}\right)(\lambda-2)^\gamma + \mathcal{O}\big((\lambda-2)^{\gamma+1}\big). \tag{2.47}$$

It furthermore holds that

$$G_\gamma(\lambda) \geq 2\mathrm{B}\left(\gamma - \frac{1}{2}, \frac{3}{2}\right)(\lambda-2)^\gamma \tag{2.48}$$

as well as

$$G_\gamma(\lambda) \geq \mathrm{B}\left(\gamma - \frac{1}{2}, 2\right)(\lambda-2)^{\gamma+\frac{1}{2}} \tag{2.49}$$

and

$$G_\gamma(\lambda) \leq \mathrm{B}\left(\gamma - \frac{1}{2}, 2\right)\lambda^{\gamma+\frac{1}{2}}. \tag{2.50}$$

For $\lambda \to \infty$ the asymptotic behaviour can be described as

$$G_\gamma(\lambda) = \mathrm{B}\left(\gamma - \frac{1}{2}, 2\right)\lambda^{\gamma+\frac{1}{2}} + \mathcal{O}\big(\lambda^{\gamma-\frac{3}{2}}\big). \tag{2.51}$$

Proof Substituting $t = (E-2)/(\lambda-2)$ in the definition of G_γ shows that

$$G_\gamma(\lambda) = (\lambda-2)^{\gamma-\frac{1}{2}} \int_0^1 \Big(\big(t(\lambda-2)+2\big)^2 - 4\Big)^{\frac{1}{2}} (1-t)^{\gamma-\frac{3}{2}}\,\mathrm{d}t$$

and the claimed asymptotic behaviour for $\lambda \to 2$ now follows from

$$\Big(\big(t(\lambda-2)+2\big)^2 - 4\Big)^{\frac{1}{2}} = 2(\lambda-2)^{\frac{1}{2}} t^{\frac{1}{2}} + \mathcal{O}\big((\lambda-2)^{\frac{3}{2}}\big).$$

Using the fact that $(E^2-4) \geq 4(E-2)$ and the same substitution as above we can furthermore compute that

$$G_\gamma(\lambda) \geq 2\int_2^\lambda (E-2)^{\frac{1}{2}}(\lambda-E)^{\gamma-\frac{3}{2}}\,\mathrm{d}E = (\lambda-2)^\gamma \int_0^1 t^{\frac{1}{2}}(1-t)^{\gamma-\frac{3}{2}}\,\mathrm{d}t\,,$$

which is precisely (2.48). Similarly we can apply the inequality $(E^2-4) \geq (E-2)^2$ and the above substitution to establish that

$$G_\gamma(\lambda) \geq \int_2^\lambda (E-2)(\lambda-E)^{\gamma-\frac{3}{2}}\,\mathrm{d}E = (\lambda-2)^{\gamma+\frac{1}{2}} \int_0^1 t(1-t)^{\gamma-\frac{3}{2}}\,\mathrm{d}t\,,$$

which proves (2.49). Substituting $t = E\lambda$ in the definition of G_γ allows us to conclude that

$$G_\gamma(\lambda) = \lambda^{\gamma+\frac{1}{2}} \int_{\frac{2}{\lambda}}^1 \left(t^2 - \frac{4}{\lambda^2}\right)^{\frac{1}{2}} (1-t)^{\gamma-\frac{3}{2}}\,\mathrm{d}t\,,$$

which can be used to show both (2.50) and (2.51). □

The asymptotic behaviour (2.51) proves that the inequalities (2.10) are optimal for large coupling. For a scalar potential b we define a reordering $b^\pm(n)$ such that $b^+(1) \geq b^+(2) \geq \cdots \geq 0$ and $b^-(1) \leq b^-(2) \leq \cdots \leq 0$. It then holds that

$$\lim_{\eta\to\infty} \frac{1}{\eta} \lambda_n^\pm(\eta b) = b^\pm(n) \tag{2.52}$$

and consequently the ratio of the left-hand side and the right-hand side of (2.10) for potential ηb converges to 1 as $\eta \to \infty$.

Inequalities (2.48) and (2.49) allow us to compare our spectral inequality (2.10) to the results of Hundertmark and Simon [42]. In their paper it is proved that in the case $A \equiv -\mathbb{I}$

the inequality

$$\sum_{j\geq 1} m_j\big(|\lambda_j|-2\big)^{\gamma} \leq d_\gamma \sum_{n\in\mathbb{Z}} \operatorname{tr}\left(|B(n)|^{\gamma+\frac{1}{2}}\right) \tag{2.53}$$

with the constant

$$d_\gamma = \frac{1}{2}\frac{\Gamma(\gamma+1)\Gamma(2)}{\Gamma(\gamma+\frac{3}{2})\Gamma(\frac{3}{2})} = \frac{1}{2}\frac{\mathrm{B}(\gamma-\frac{1}{2},2)}{\mathrm{B}(\gamma-\frac{1}{2},\frac{3}{2})} = 2L^{\mathrm{cl}}_{\gamma,1}$$

holds for all $\gamma \geq \frac{1}{2}$. Here, $L^{\mathrm{cl}}_{\gamma,1}$ is the semi-classical Lieb–Thirring constant. From (2.48) we can conclude that

$$\frac{1}{d_\gamma}\sum_{j\geq 1} m_j\big(|\lambda_j|-2\big)^{\gamma} \leq \frac{1}{\mathrm{B}(\gamma-\frac{1}{2},2)}\sum_{j\geq 1} m_j G_\gamma(|\lambda_j|) \leq \sum_{n\in\mathbb{Z}} \operatorname{tr}\left(|B(n)|^{\gamma+\frac{1}{2}}\right), \tag{2.54}$$

which shows that inequality (2.10) is indeed better than (2.53). From (2.47) we can conclude that for eigenvalues $|\lambda_j| \to 2$ approaching the essential spectrum the two inequalities have the same asymptotic behaviour. In their paper [42], Hundertmark and Simon also proved that for $\gamma \geq \frac{1}{2}$

$$\sum_{j\geq 1} m_j(|\lambda_j|-2)^{\gamma+\frac{1}{2}} \leq \sum_{n\in\mathbb{Z}} \operatorname{tr}\left(|B(n)|^{\gamma+\frac{1}{2}}\right), \tag{2.55}$$

which was found to be optimal for large coupling. Using (2.49) we obtain that

$$\sum_{j\geq 1} m_j(|\lambda_j|-2)^{\gamma+\frac{1}{2}} \leq \frac{1}{\mathrm{B}(\gamma-\frac{1}{2},2)}\sum_{j\geq 1} m_j G_\gamma(|\lambda_j|) \leq \sum_{n\in\mathbb{Z}} \operatorname{tr}\left(|B(n)|^{\gamma+\frac{1}{2}}\right), \tag{2.56}$$

which leads to the conclusion that (2.10) is also more precise than (2.55). From (2.51) it follows that in the limit $|\lambda_j| \to \infty$ the two inequalities show the same asymptotic behaviour.

For choices of γ which are not half-integers, the integral in the definition of $G_\gamma(\lambda)$ can unfortunately not be computed explicitly. We are particularly interested in the case $\gamma = 1$. We can at least numerically compute $G_1(\lambda)$ for different values of λ. In Figure 2.1 we compare the two ratios

$$R_1(\lambda) = \left(\frac{G_1(\lambda)}{\mathrm{B}(\frac{1}{2},2)}\right) \Big/ \left(\frac{\lambda-2}{d_1}\right), \qquad R_2(\lambda) = \left(\frac{G_1(\lambda)}{\mathrm{B}(\frac{1}{2},2)}\right) \Big/ (\lambda-2)^{\frac{3}{2}}.$$

From (2.54), (2.56) it follows that $R_1(\lambda) \geq 1$ and $R_2(\lambda) \geq 1$ which is clearly visualised in the plot. The figure also indicates the asymptotic behaviours (2.47) and (2.51), which imply that $\lim_{\lambda\to 2} R_1(\lambda) = \lim_{\lambda\to\infty} R_2(\lambda) = 1$.

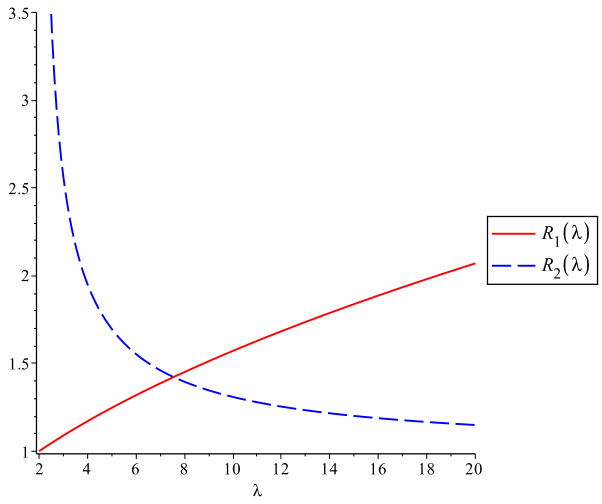


Figure 2.1: Comparison of the governing terms in the spectral inequalities

Theorem 2.5.1 is not expected to be sharp because of the additional factor of $3^{\gamma-\frac{1}{2}}$. The proof of this inequality uses the method that was discussed at the beginning of Section 2.1. The preliminary bound

$$\begin{aligned}&\sum_{j\geq 1}\int_2^{|\lambda_j|}(E^2-4)^{\frac{1}{2}}(|\lambda_j|-E)^{\gamma-\frac{3}{2}}\,\mathrm{d}E\\&\leq \mathrm{B}\Big(\gamma-\frac{1}{2},2\Big)\sum_{n\in\mathbb{Z}}\Big(\big(b(n)_+ + |a(n-1)+1| + |a(n)+1|\big)^{\gamma+\frac{1}{2}}\\&\qquad\qquad + \big(b(n)_- + |a(n-1)+1| + |a(n)+1|\big)^{\gamma+\frac{1}{2}}\Big)\end{aligned} \tag{2.57}$$

is used in this proof. Since (2.49) holds and since (2.52) remains true for Jacobi operators with off-diagonal entries $a(n)$ which are independent of η, the above inequality is found to be optimal for large coupling of b.

Chapter 3

Approximation of a Schrödinger Operator on the Continuum

We will use the established inequalities of Chapter 2 to prove analogous results for a Schrödinger operator $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$ on $L^2(\mathbb{R})$. In particular, we will provide new proofs for the sharp Lieb–Thirring bounds (1.5) in one dimension for $\gamma = \frac{1}{2}$ and $\gamma = \frac{3}{2}$.

We will show that (2.2) with constant $a \equiv -1$ is sufficient to prove the sharp Lieb–Thirring inequality on $L^2(\mathbb{R})$ for $\gamma = \frac{1}{2}$. To give further merit to the fact that the result of Hundertmark and Simon is also asymptotically optimal for general off-diagonal entries, we will show that restricting (2.2) to vanishing potentials $b \equiv 0$ also yields the sharp Lieb–Thirring constant $L_{1/2,1}$ on $L^2(\mathbb{R})$.

Subsequently we will show that (2.6) yields the sharp Lieb–Thirring constant $L_{3/2,1}$ on $L^2(\mathbb{R})$. Unlike in the proof for $\gamma = \frac{1}{2}$, it will not be sufficient to restrict ourselves to discrete Schrödinger operators in the approximation of the Schrödinger operator on the continuum. The terms depending on b and the terms depending on a in (2.6) will play an equally important role. For this reason, the new inequalities (2.10) for $\frac{1}{2} < \gamma < \frac{3}{2}$, which we only managed to prove for discrete Schrödinger operators, will not yield the sharp Lieb–Thirring constants $L_{\gamma,1}$ on $L^2(\mathbb{R})$. The inequalities of Theorem 2.5.1 will not lead to any improvement as they were only derived from (2.10) by means of a perturbation argument. Making use of an additional symmetry argument, we will see that at least in the case $\gamma = \frac{3}{2}$ it is sufficient to consider (2.6) for Jacobi operators with $b \equiv 0$ to derive the sharp constant $L^{\mathrm{cl}}_{3/2,1}$ on the continuum.

To carry out the approximations, we follow [76] where the following theorem is proved.

Theorem 3.0.2 *[76, Theorem 2.3] Let $(E, \|\cdot\|)$ be a Banach Space and let E_1 be a dense linear subspace. Let $(F_k, \|\cdot\|_k)$ be a sequence of Banach spaces such that for every $k \in \mathbb{N}$ there exists a (not necessarily bounded) linear operator $P_k : E_1 \to F_k$ such that $\lim_{k\to\infty} \|P_k f\|_k = \|f\|$ for all $f \in E_1$. Consider a densely defined closed operator $\big(H, \mathrm{dom}(H)\big)$ on E with domain $\mathrm{dom}(H)$ and let $E_0 \subset E_1$ be a core of H such that $H(E_0) \subset E_1$. For each $k \in \mathbb{N}$ let $\big(H_k, \mathrm{dom}(H_k)\big)$ be a densely defined operator on F_k such that $P_k(E_1) \subset \mathrm{dom}(H_k)$ and $\lim_{k\to\infty} \|H_k P_k f - P_k H f\|_k = 0$ for all $f \in E_0$. If there exists an $M > 0$ such that*

$$\big\|(H_k - \lambda)^{-1}\big\| \leq \frac{M}{\mathrm{dist}\big(\lambda, \sigma(H_k)\big)} \tag{3.1}$$

for all $\lambda \in \rho(H_k)$ and all $k \in \mathbb{N}$, then for any compact set $K \subset \mathbb{C}$

$$\lim_{k\to\infty} \mathrm{dist}\big(\sigma_a(H) \cap K, \sigma(H_k)\big) = 0\,.$$

Here, the distance between a bounded set $X \subset \mathbb{C}$ and a nonempty set $Y \subset \mathbb{C}$ is defined by

$$\mathrm{dist}\big(X, Y\big) = \sup_{x\in X} \inf_{y\in Y} |x - y|$$

and $\sigma_a(H)$ denotes the approximate point spectrum of H, which consists of all $\lambda \in \mathbb{C}$ for which there exists a sequence of $f_1, f_2, \cdots \in \mathrm{dom}(H)$ that satisfies $\|f_n\| = 1$ for all $n \in \mathbb{N}$ and $\lim_{n\to\infty} \|Hf_n - \lambda f_n\| = 0$.

3.1 Approximation by Discrete Schrödinger Operators

In our case $E = L^2(\mathbb{R})$ and $H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$. For the moment we shall assume that the potential is smooth and compactly supported, $V \in \mathcal{C}_c^\infty(\mathbb{R})$. The operator H is self-adjoint on the domain $\mathrm{dom}(H) = H^2(\mathbb{R})$, the Sobolev space of functions in $L^2(\mathbb{R})$ that are twice weakly differentiable. We choose $E_1 = E_0 = \mathcal{C}_c^\infty(\mathbb{R})$, which is well-known to form a core of H, and note that $H(E_0) \subset E_1$. The Banach spaces F_k are chosen to be $\ell^2(\mathbb{Z})$ with the scalar product

$$(c, d)_k = \frac{1}{k} \sum_{n\in\mathbb{Z}} c(n)\overline{d(n)}$$

and the operator $P_k : E_1 \to F_k$ is defined via

$$(P_k f)(n) = f\Big(\frac{n}{k}\Big)\,, \quad n \in \mathbb{Z}\,,$$

for all $f \in E_1$. Note that this operator is well-defined as the compact support of f guarantees that $\|P_k f\|_k$ is given by a finite sum. Furthermore, by the definition of Riemann integrability, it holds that

$$\lim_{k\to\infty} \|P_k f\|_k^2 = \lim_{k\to\infty} \frac{1}{k} \sum_{n\in\mathbb{Z}} \Big| f\Big(\frac{n}{k}\Big)\Big|^2 = \int_{\mathbb{R}} |f(x)|^2 \,\mathrm{d}x = \|f\|_{L^2}^2 \,.$$

The operator H_k is now defined on F_k as

$$(H_k u)(n) = k^2\big(-u(n+1) + 2u(n) - u(n-1)\big) + V\Big(\frac{n}{k}\Big)\, u(n)\,.$$

Due to the compact support of the potential, H_k is a bounded, self-adjoint operator on F_k. Thus the operator is in particular normal and hence (3.1) holds with $M = 1$. It remains to show that $\lim_{k\to\infty} \|H_k P_k f - P_k H f\|_k = 0$ for all $f \in E_0$. Let $N \in \mathbb{N}$ be sufficiently large such that $\mathrm{supp}(f) \subset [-N, N]$. We observe that

$$\begin{aligned}
&\|H_k P_k f - P_k H f\|_k^2 \\
&= \frac{1}{k} \sum_{n=-Nk-1}^{Nk+1} \left| k^2 \left(-f\Big(\frac{n+1}{k}\Big) + 2f\Big(\frac{n}{k}\Big) - f\Big(\frac{n-1}{k}\Big)\right) + f''\Big(\frac{n}{k}\Big)\right|^2 .
\end{aligned}$$

As $f \in \mathcal{C}_c^\infty(\mathbb{R})$, Taylor's theorem shows that there exists a constant $C > 0$ depending only on f such that every summand in the above sum is smaller than $C\frac{1}{k^4}$. This proves that

$$\|H_k P_k f - P_k H f\|_k^2 \leq \frac{1}{k^5}(2Nk + 3)$$

where the right-hand side converges to zero as $k \to \infty$. Thus all the assumptions of Theorem 3.0.2 are satisfied.

Denote by $\mu_1 < \cdots < \mu_N < 0$ the finite sequence of negative eigenvalues of H in increasing order. Choosing $K = [\mu_1, \mu_N] \subset \mathbb{R}$, Theorem 3.0.2 states that

$$\lim_{k\to\infty} \max_{j=1,\dots,N} \inf_{\lambda\in\sigma(H_k)} |\mu_j - \lambda| = 0\,. \tag{3.2}$$

Note that $W_k = k^{-2}H_k - 2$ is a discrete Schrödinger operator of the form (2.1) with $a_k \equiv -1$ and scalar potential $b_k(n) = k^{-2}V(n/k)$. Its essential spectrum is given by $[-2, 2]$ and it has a finite sequence of eigenvalues outside of this interval. These eigenvalues satisfy the spectral inequalities discussed in the previous chapter, in particular the scalar versions of (2.39) and (2.10). If we denote by $\lambda_{k,j}$ the discrete eigenvalues of H_k the above observations let us conclude that each $\lambda_{k,j}$ is in the complement of the interval $k^2[0, 4]$ and that

$$\sum_{j\geq 1} \left((k^{-2}\lambda_{k,j} - 2)^2 - 4\right)^{\frac{1}{2}} \leq \frac{1}{k^2} \sum_{n\in\mathbb{Z}} \left|V\left(\frac{n}{k}\right)\right|$$

as well as

$$\sum_{j\geq 1} G_\gamma(|k^{-2}\lambda_{k,j} - 2|) \leq \mathrm{B}\left(\gamma - \frac{1}{2}, 2\right) \frac{1}{k^{2\gamma+1}} \sum_{n\in\mathbb{Z}} \left|V\left(\frac{n}{k}\right)\right|^{\gamma+\frac{1}{2}}$$

for all $\gamma > \frac{1}{2}$. If we sum only over all the negative eigenvalues $\lambda^-_{k,j}$ of H_k then

$$\sum_{j\geq 1} \left((k^{-2}\lambda^-_{k,j} - 2)^2 - 4\right)^{\frac{1}{2}} \leq \frac{1}{k^2} \sum_{n\in\mathbb{Z}} V\left(\frac{n}{k}\right)_- \tag{3.3}$$

and for $\gamma > \frac{1}{2}$

$$\sum_{j\geq 1} G_\gamma(|k^{-2}\lambda^-_{k,j} - 2|) \leq \mathrm{B}\left(\gamma - \frac{1}{2}, 2\right) \frac{1}{k^{2\gamma+1}} \sum_{n\in\mathbb{Z}} V\left(\frac{n}{k}\right)_-^{\gamma+\frac{1}{2}} . \tag{3.4}$$

A simple calculation for negative $\lambda < 0$ shows that

$$\left((k^{-2}\lambda - 2)^2 - 4\right)^{\frac{1}{2}} = k^{-1}(k^{-2}\lambda^2 - 4\lambda)^{\frac{1}{2}}$$

and consequently inequality (3.3) can be written as

$$\sum_{j\geq 1} \left(k^{-2}(\lambda^-_{k,j})^2 - 4\lambda_{k,j}\right)^{\frac{1}{2}} \leq \frac{1}{k} \sum_{n\in\mathbb{Z}} V\left(\frac{n}{k}\right)_- .$$

From (3.2) we conclude that the negative eigenvalues $\lambda^-_{k,j}$ approximate the eigenvalues $\mu_1, \ldots, \mu_N$ as $k \to \infty$. Thus, taking the limit $k \to \infty$ in the above spectral inequality and

using the definition of Riemann integrability we arrive at

$$\sum_{j\geq 1} |\mu_j|^{\frac{1}{2}} \leq \frac{1}{2} \int_{\mathbb{R}} V(x)_- \, \mathrm{d}x \,,$$

which is the best possible bound. Using a further approximation argument, the assumption $V \in \mathcal{C}_c^\infty(\mathbb{R})$ can be generalised to the weaker $V \in L^1(\mathbb{R})$.

Using the substitution $s = k^2(E-2)/|\lambda|$ it is straightforward to show that for $\gamma > \frac{1}{2}$ and $\lambda < 0$ we can write

$$G_\gamma(|k^{-2}\lambda - 2|) = G_\gamma(2 + k^{-2}|\lambda|) = \frac{1}{k^{2\gamma}} |\lambda|^\gamma \int_0^1 s^{\frac{1}{2}} (1-s)^{\gamma - \frac{3}{2}} (4 + sk^{-2}|\lambda|)^{\frac{1}{2}} \, \mathrm{d}s \,.$$

Together with (3.4) this allows us to conclude that

$$\sum_{j\geq 1} |\lambda_{k,j}^-|^\gamma \int_0^1 s^{\frac{1}{2}} (1-s)^{\gamma-\frac{3}{2}} (4 + sk^{-2}|\lambda_{k,j}^-|)^{\frac{1}{2}} \, \mathrm{d}s \leq \mathrm{B}\left(\gamma - \frac{1}{2}, 2\right) \frac{1}{k} \sum_{n\in\mathbb{Z}} V\left(\frac{n}{k}\right)_-^{\gamma+\frac{1}{2}}.$$

In the limit $k \to \infty$ this inequality yields

$$\sum_{j\geq 1} |\mu_j|^\gamma \leq \frac{\mathrm{B}(\gamma - \frac{1}{2}, 2)}{2\mathrm{B}(\gamma - \frac{1}{2}, \frac{3}{2})} \int_{\mathbb{R}} V(x)_-^{\gamma+\frac{1}{2}} \, \mathrm{d}x = 2L^{\mathrm{cl}}_{\gamma,1} \int_{\mathbb{R}} V(x)_-^{\gamma+\frac{1}{2}} \, \mathrm{d}x \,,$$

which is not the sharp result. Note that using (2.3) instead of (2.10) leads to the same result, as the difference between these two inequalities vanishes for small eigenvalues. As mentioned before, for $\gamma \geq 1$ the constant $d_\gamma = 2L^{\mathrm{cl}}_{\gamma,1}$ can be improved to $\frac{\pi}{\sqrt{3}} L^{\mathrm{cl}}_{\gamma,1}$ [63]. This proves the result of [25] on $L^2(\mathbb{R})$ from our approximation. In order to get sharp inequalities for $\gamma \geq \frac{3}{2}$, we will use a different approximation of H in the next section.

3.2 Approximation by Jacobi Operators

One could expect better results by approximating the operator on the continuum by discrete operators whose off-diagonal entries $a_k(n)$ are not restricted to be -1. Let the vector spaces E_0, E_1, F_k and the linear operators P_k be defined as in the previous section. Take $c \in [0,1]$

and set $d = (1-c)/2$ such that $c + 2d = 1$. We now define the operator H_k on F_k as

$$\begin{aligned}(H_k u)(n) &= k^2\left(-u(n-1) + 2u(n) - u(n+1)\right) \\ &\quad + cV\Big(\frac{n}{k}\Big)\,u(n) + dV\left(\frac{n-1}{k}\right)u(n-1) + dV\Big(\frac{n}{k}\Big)\,u(n+1)\,.\end{aligned} \tag{3.5}$$

Suppose that $f \in E_0$ and that $N \in \mathbb{N}$ is sufficiently large such that $[-N, N]$ covers both the support of V and the support of f. Then it holds that

$$\begin{aligned}&\|H_k P_k f - P_k H f\|_k^2 \\ &\leq \frac{1}{k}\sum_{n=-Nk+1}^{Nk+1}\Bigg(\left|k^2\left(-f\left(\frac{n+1}{k}\right) + 2f\Big(\frac{n}{k}\Big) - f\left(\frac{n-1}{k}\right)\right) + f''\Big(\frac{n}{k}\Big)\right| \\ &\quad + \left|(c-1)V\Big(\frac{n}{k}\Big)\,f\Big(\frac{n}{k}\Big) + dV\left(\frac{n-1}{k}\right)f\left(\frac{n-1}{k}\right) + dV\Big(\frac{n}{k}\Big)\,f\left(\frac{n+1}{k}\right)\right|\Bigg)^2.\end{aligned}$$

As discussed previously, Taylor's theorem and the boundedness of f yield the existence of a constant C_1 such that

$$\left|k^2\left(-f\left(\frac{n+1}{k}\right) + 2f\Big(\frac{n}{k}\Big) - f\left(\frac{n-1}{k}\right)\right) + f''\Big(\frac{n}{k}\Big)\right| \leq C_1\frac{1}{k^2}\,. \tag{3.6}$$

To find a similar bound for the second term, we first note that by Taylor's theorem there exists $\xi \in (n/k - 1/k, n/k)$ such that

$$V\left(\frac{n-1}{k}\right) = V\Big(\frac{n}{k}\Big) - \frac{1}{k}V'(\xi)\,.$$

This lets us conclude that

$$\begin{aligned}&\left|(c-1)V\Big(\frac{n}{k}\Big)\,f\Big(\frac{n}{k}\Big) + dV\left(\frac{n-1}{k}\right)f\left(\frac{n-1}{k}\right) + dV\Big(\frac{n}{k}\Big)\,f\left(\frac{n+1}{k}\right)\right| \\ &\leq \left|V\Big(\frac{n}{k}\Big)\right|\left|(c-1)f\Big(\frac{n}{k}\Big) + df\left(\frac{n-1}{k}\right) + df\left(\frac{n+1}{k}\right)\right| + \frac{1}{k}\left|V'(\xi)f\left(\frac{n-1}{k}\right)\right|,\end{aligned} \tag{3.7}$$

where the last term can be bounded by C_2/k with the constant $C_2 > 0$ depending only on V and f since $V, f \in \mathcal{C}_c^\infty(\mathbb{R})$. By Taylor's theorem there also exist $\xi_- \in (n/k - 1/k, n/k)$

and $\xi_+ \in (n/k, n/k + 1/k)$ such that

$$f\left(\frac{n \pm 1}{k}\right) = f\left(\frac{n}{k}\right) \pm \frac{1}{k} f'(\xi_\pm)\,.$$

This allows us to continue (3.7) as

$$\begin{aligned}
&\left|(c-1)V\left(\frac{n}{k}\right) f\left(\frac{n}{k}\right) + dV\left(\frac{n-1}{k}\right) f\left(\frac{n-1}{k}\right) + dV\left(\frac{n}{k}\right) f\left(\frac{n+1}{k}\right)\right| \\
&\leq \left|V\left(\frac{n}{k}\right)\right| \frac{d}{k} \left|f'(\xi_+) - f'(\xi_-)\right| + C_2 \frac{1}{k} \\
&\leq C_3 \frac{1}{k}\,,
\end{aligned}$$

where $C_3 > 0$ is a constant depending only on V and f. Together with (3.6) we have shown that

$$\|H_k P_k f - P_k H f\|_k^2 \leq \frac{1}{k}(2Nk + 3)\left(C_1 \frac{1}{k^2} + C_3 \frac{1}{k}\right)^2,$$

where the right-hand side clearly converges to zero as $k \to \infty$. Thus all the assumptions of Theorem 3.0.2 are satisfied.

The operator $W_k = k^{-2} H_k - 2$ is of the form (2.1) with potential $b_k(n) = ck^{-2} V(n/k)$ and off-diagonal terms $a_k(n) = -1 + dk^{-2} V(n/k)$. Note that clearly $a_k(n) < 0$ if k is sufficiently large. Let $\lambda_{k,j}^-$ be the negative eigenvalues of H_k. Inequality (2.6) now holds for the eigenvalues of W_k and in particular if we only consider the negative eigenvalues. Recalling (2.40) this can be written as

$$2 \sum_{j \geq 1} G_{\frac{3}{2}}(|k^{-2} \lambda_{k,j}^- - 2|) \leq \sum_{n \in \mathbb{Z}} b_k(n)^2 + 2 \sum_{n \in \mathbb{Z}} \left(a_k(n)^2 - 1 - \log a_k(n)^2\right).$$

We now apply (2.48) and insert the definitions of $a_k(n)$ and $b_k(n)$ to conclude that

$$\begin{aligned}
&4\mathrm{B}\left(1, \frac{3}{2}\right) \sum_{j \geq 1} |\lambda_{k,j}^-|^{\frac{3}{2}} \\
&\leq \sum_{n \in \mathbb{Z}} \left(\frac{c^2 + 2d^2}{k} V\left(\frac{n}{k}\right)^2 - 4dk V\left(\frac{n}{k}\right) - 2k^3 \log\left(1 - \frac{2d}{k^2} V\left(\frac{n}{k}\right) + \frac{d^2}{k^4} V\left(\frac{n}{k}\right)^2\right)\right).
\end{aligned}$$

Using the Taylor expansion $\log(1 + x) = x - x^2/2 + \mathcal{O}(x^3)$ for small $|x|$ and (3.2) as well

as the Riemann integrability of V, we can let $k \to \infty$ to obtain

$$\sum_{j\geq 1} |\mu_j|^{\frac{3}{2}} \leq \frac{1}{4\mathrm{B}(1,\frac{3}{2})}(c^2+4d^2)\int_{\mathbb{R}} V(x)^2\,\mathrm{d}x = 2L^{\mathrm{cl}}_{\frac{3}{2},1}(c^2+4d^2)\int_{\mathbb{R}} V(x)^2\,\mathrm{d}x\,.$$

We can minimise the right-hand side with respect to $c \in [0,1]$ and it is straightforward to prove that the minimum is attained at $c = \frac{1}{2}$. This yields

$$\sum_{j\geq 1} |\mu_j|^{\frac{3}{2}} \leq L^{\mathrm{cl}}_{\frac{3}{2},1}\int_{\mathbb{R}} V(x)^2\,\mathrm{d}x\,,$$

which by continuity can be shown to hold under the more general assumption $V \in L^2(\mathbb{R})$. Finally, the Min–Max principle implies that V on the right-hand side of the inequality can be replaced by V_-, yielding the sharp Lieb–Thirring inequality

$$\sum_{j\geq 1} |\mu_j|^{\frac{3}{2}} \leq L^{\mathrm{cl}}_{\frac{3}{2},1}\int_{\mathbb{R}} V(x)_-^2\,\mathrm{d}x\,.$$

The Aizenman–Lieb principle extends this result immediately to higher powers $\gamma \geq \frac{3}{2}$.

We can also try to obtain better bounds for $\frac{1}{2} < \gamma < \frac{3}{2}$ using this approximation and (2.3). If we sum only over all the negative eigenvalues in (2.3) then the constant 4 can be replaced by 2 as we can easily see from the perturbation argument detailed in Section 2.2. This yields that for all $\gamma \geq \frac{1}{2}$

$$\begin{aligned}\sum_{j\geq 1} |\lambda^-_{k,j}|^{\gamma} &\leq c_\gamma\left(\frac{d^{\gamma+\frac{1}{2}}}{k}\sum_{n\in\mathbb{Z}}\left|V\Big(\frac{n}{k}\Big)\right|^{\gamma+\frac{1}{2}} + \frac{2d^{\gamma+\frac{1}{2}}}{k}\sum_{n\in\mathbb{Z}}\left|V\Big(\frac{n}{k}\Big)\right|^{\gamma+\frac{1}{2}}\right)\\ &= c_\gamma\left(c^{\gamma+\frac{1}{2}}+2d^{\gamma+\frac{1}{2}}\right)\frac{1}{k}\sum_{n\in\mathbb{Z}}\left|V\Big(\frac{n}{k}\Big)\right|^{\gamma+\frac{1}{2}}.\end{aligned}$$

Letting $k \to \infty$ and using (3.2), we arrive at

$$\sum_{j\geq 1} |\mu_j|^{\gamma} \leq 2L^{\mathrm{cl}}_{\gamma,1}3^{\gamma-\frac{1}{2}}\left(c^{\gamma+\frac{1}{2}}+2d^{\gamma+\frac{1}{2}}\right)\int_{\mathbb{R}} |V(x)|^{\gamma+\frac{1}{2}}\,\mathrm{d}x\,.$$

We can now minimise the function $c^{\gamma+\frac{1}{2}} + 2d^{\gamma+\frac{1}{2}}$ on the right-hand side with respect to $c \in [0,1]$. If $\gamma = \frac{1}{2}$ we observe that the function is constant 1 and consequently the minimum is attained at any $c \in [0,1]$. Thus, no matter which approximation we choose

exactly, we will always get the sharp Lieb–Thirring constant $2L^{\mathrm{cl}}_{1/2,1}$. For $\gamma > \frac{1}{2}$ we find that the minimum is attained at $c = \frac{1}{3}$. Consequently we obtain that

$$\sum_{j\geq 1} |\mu_j|^\gamma \leq 2L^{\mathrm{cl}}_{\gamma,1} \int_{\mathbb{R}} |V(x)|^{\gamma+\frac{1}{2}} \,\mathrm{d}x\,,$$

which is unfortunately exactly the same result as in the previous section. This is not surprising, as Hundertmark and Simon derived the inequalities (2.3) from the result for constant diagonal terms using a perturbation argument. Similarly the inequalities of Theorem 2.5.1 as well as the inequalities (2.57) only yield the constants $2L^{\mathrm{cl}}_{\gamma,1}$ on the real line. To obtain the best possible Lieb–Thirring constants for $\frac{1}{2} < \gamma < \frac{3}{2}$ from our approximation method, it would first be necessary to establish the correct terms depending on $a(n)$ on the right-hand side of (2.10) such that optimisers exist or to further improve inequality (2.3) in the special case of a discrete Schrödinger operator.

3.3 Approximation by Jacobi Operators with Vanishing Potential

As we have seen in the previous section, the spectral inequality (2.6) can be used to prove the sharp Lieb–Thirring constant $L^{\mathrm{cl}}_{3/2,1}$ for the operator $H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$ on the real line. The approximating operators were chosen to be Jacobi operators (3.5) . The sharp Lieb–Thirring constant $L^{\mathrm{cl}}_{3/2,1}$ was found by choosing $c = \frac{1}{2}$. In particular, it was not sufficient to restrict the approximating operators to discrete Schrödinger operators ($a_k \equiv -1$ or equivalently $c = 1$) which only yielded the constant $2L^{\mathrm{cl}}_{3/2,1}$ on $\mathbb{R}$. However, exploring the symmetry of the spectrum, it is possible to derive the sharp constant $L^{\mathrm{cl}}_{3/2,1}$ using approximation by Jacobi operators with vanishing potential ($b_k \equiv 0$ or equivalently $c = 0$).

To this end we simply note that for a Jacobi operator W with $b \equiv 0$ the spectrum is symmetric with respect to 0. This can be seen by a simple computation (see Subsection 2.3.2) which shows that if ψ is an eigenfunction to the eigenvalue λ, then $\psi'(n) := (-1)^n\psi(n)$ is an eigenfunction to the eigenvalue $-\lambda$. From (2.6) we obtain that

$$\sum_{j\geq 1} \int_2^{|\lambda_j|} (|\lambda_j|^2 - E)^{\frac{1}{2}} \,\mathrm{d}E \leq \sum_{n\in\mathbb{Z}} \left(a(n)^2 - 1 - \log a(n)^2\right)$$

and due to the symmetry of the eigenvalues we can conclude that if we only sum over the

negative eigenvalues λ_j^- then

$$\sum_{j\geq 1}\int_2^{|\lambda_j^-|}(|\lambda_j^-|^2-E)^{\frac{1}{2}}\,\mathrm{d}E\leq\frac{1}{2}\sum_{n\in\mathbb{Z}}\left(a(n)^2-1-\log a(n)^2\right).$$

We have thus improved the inequality by a factor of $1/2$. Using the approximating Jacobi operators (3.5) with vanishing potential ($b_k\equiv 0$ or equivalently $c=0$) and repeating the computations of the preceding Section 3.2, the negative eigenvalues $\mu_1<\mu_2<\cdots\leq 0$ of H can be bounded by

$$\sum_{j\geq 1}|\mu_j|^{\frac{3}{2}}\leq\frac{1}{8\mathrm{B}(1,\frac{3}{2})}\int_{\mathbb{R}}V(x)^2\,\mathrm{d}x=L^{\mathrm{cl}}_{\frac{3}{2},1}\int_{\mathbb{R}}V(x)^2\,\mathrm{d}x\,,$$

which is the sharp result.

We cannot use this symmetry argument to improve the Lieb–Thirring constants obtained from (2.3) in Section 3.2. The reason is that in our computations we have already replaced the constant 4 in front to the off-diagonal terms by 2 using the fact that we are only interested in the sum of the negative eigenvalues.

3.4 Interpolation between the Inequalities

We have proved that the spectral inequalities (2.2) and (2.6) can be used to establish sharp Lieb–Thirring inequalities on the real line for $\gamma=\frac{1}{2}$ and for $\gamma=\frac{3}{2}$, respectively. We did not obtain sharp constants for $\frac{1}{2}<\gamma<\frac{3}{2}$ since the inequalities (2.10) were only derived for $a\equiv -1$. In this section we aim use interpolation to derive spectral inequalities for the Jacobi operator that that lie in-between (2.2) and (2.6).

To make the computation easier, we consider (2.4) with $\gamma=\frac{1}{2}$

$$\sum_{j\geq 1}(|\lambda_j^-|-2)^{\frac{1}{2}}\leq 2L^{\mathrm{cl}}_{\frac{1}{2},1}\left(\sum_{n\in\mathbb{Z}}|b(n)|+2\sum_{n\in\mathbb{Z}}|a(n)+1|\right)\tag{3.8}$$

instead of (2.2). This inequality has the advantage that the left-hand side and the right-hand side can be written in terms of ℓ^p norms. We want to apply a similar simplification to (2.6)

and note that

$$x^2 - 1 - \log x^2 \leq 2(x+1)^2$$

for all $x \leq -1$. This allows us to conclude that if $a(n) \leq -1$ for all $n \in \mathbb{Z}$, then

$$\sum_{j\geq 1}(|\lambda_j^-| - 2)^{\frac{3}{2}} \leq 2L^{\mathrm{cl}}_{\frac{3}{2},1}\left(\sum_{n\in\mathbb{Z}}|b(n)|^2 + 4\sum_{n\in\mathbb{Z}}|a(n)+1|^2\right). \tag{3.9}$$

Note that although we have simplified the spectral inequalities, (3.8) and (3.9) can be used to prove the sharp Lieb–Thirring constants $2L^{\mathrm{cl}}_{1/2,1}$ and $L^{\mathrm{cl}}_{3/2,1}$ on the real line. We will interpolate between (3.8) and (3.9) whereby we will closely follow [74], where interpolation between Lieb–Thirring inequalities on the continuum was undertaken.

3.4.1 Interpolation Theory

For a rigorous description of interpolation theory we refer to [8]. For $p_0, p_1 > 0$ and for a sequence $u \in \ell^{p_0}(\mathbb{Z}) + \ell^{p_1}(\mathbb{Z})$ the K-function is defined as

$$K(u,t,p_0,p_1) = \inf_{\substack{u=u_0+u_1\\ u_j\in\ell^{p_j}}}\left(\|u_0\|^{p_0}_{\ell^{p_0}} + t\,\|u_1\|^{p_1}_{\ell^{p_1}}\right),$$

where $t \geq 0$. Here and in the remainder of this chapter we will often use the shortened notation ℓ^p instead of $\ell^p(\mathbb{Z})$. If $p < 1$ then $\|u\|^p_{\ell^p}$ denotes the quasi-norm $\|u\|^p_{\ell^p} = \sum_{n\in\mathbb{Z}}|u(n)|^p$. Note that the commonly used definition of K involves only the terms $\|u_0\|_{\ell^{p_0}}$ and $\|u_1\|_{\ell^{p_1}}$ without the powers p_0 and p_1. The so-called 'power theorem' (see e.g. [8, Theorem 3.11.6]) allows us to include the powers p_0 and p_1 in the definition of K. This is important for our application, as the inequalities (3.8) and (3.9) involve powers of quasi-norms on ℓ^p spaces. For functions $h : (0,\infty) \to [0,\infty)$ we consider the functional

$$\Phi_{\eta,1}(h) = \int_0^\infty t^{-\eta-1}h(t)\,\mathrm{d}t$$

with $\eta \in (0,1)$. Clearly $\Phi_{\eta,1}(h_1) \leq \Phi_{\eta,1}(h_2)$ if $h_1(t) \leq h_2(t)$ and following a remark in [74] and the computations in [8, p. 111] we can prove the following result.

Lemma 3.4.1 *With $p = (1-\eta)p_0 + \eta p_1$ it holds that*

$$\Phi_{\eta,1}\big(K(u,\cdot,p_0,p_1)\big) = \Theta(\eta,p_0,p_1)\,\|u\|_{\ell^p}^p$$

where

$$\Theta(\eta,p_0,p_1) = \int_0^\infty t^{-\eta-1} \inf_{y_0+y_1=1} \big(|y_0|^{p_0} + t|y_1|^{p_1}\big)\,\mathrm{d}t\,.$$

Proof We begin by computing that

$$\begin{aligned}
\inf_{\substack{u=u_0+u_1,\\ u_j\in\ell^{p_j}}} (\|u_0\|_{\ell^{p_0}}^{p_0} + t\,\|u_1\|_{\ell^{p_2}}^{p_1}) &= \inf_{\substack{u=u_0+u_1,\\ u_j\in\ell^{p_j}}} \sum_{n\in\mathbb{Z}} (|u_0(n)|^{p_0} + t|u_1(n)|^{p_1}) \\
&= \sum_{n\in\mathbb{Z}} \inf_{u(n)=u_0(n)+u_1(n)} (|u_0(n)|^{p_0} + t|u_1(n)|^{p_1}) \\
&= \sum_{n\in\mathbb{Z}} |u(n)|^{p_0} \inf_{1=y_0+y_1} \big(|y_0|^{p_0} + t|u(n)|^{p_1-p_0}|y_1|^{p_1}\big)\,.
\end{aligned}$$

Note that the second equality is not trivial. We fist observe that numbers $d_0(n), d_1(n)$ can be chosen such that

$$|d_0(n)|^{p_0} + t|d_1(n)|^{p_1} = \inf_{u(n)=u_0(n)+u_1(n)} (|u_0(n)|^{p_0} + t|u_1(n)|^{p_1})$$

since the expression over which we take the infinum grows to infinity if $|u_0(n)|$ or $|u_1(n)|$ becomes large. We then note that

$$\sum_{n\in\mathbb{Z}} |d_0(n)|^{p_0} \le \inf_{\substack{u=u_0+u_1,\\ u_j\in\ell^{p_j}}} (\|u_0\|_{\ell^{p_0}}^{p_0} + t\,\|u_1\|_{\ell^{p_1}}^{p_1}) < \infty$$

and that a similar results holds for d_1. Thus the interchange of infinum and summation in the first computation is justified. We now apply $\Phi_{\eta,1}$ to the derived identity and use the substitution $s = t|u(n)|^{p_1-p_0}$ to obtain that

$$\begin{aligned}
\Phi_{\eta,1}\big(K(u,\cdot,p_0,p_1)\big) &= \sum_{n\in\mathbb{Z}} |u(n)|^{p_0} \int_0^\infty t^{-\eta-1} \inf_{1=y_0+y_1} \big(|y_0|^{p_0} + t|u(n)|^{p_1-p_0}|y_1|^{p_1}\big)\,\mathrm{d}t \\
&= \sum_{n\in\mathbb{Z}} |u(n)|^{p} \int_0^\infty s^{-\eta-1} \inf_{1=y_0+y_1} (|y_0|^{p_0} + s|y_1|^{p_1})\,\mathrm{d}s\,,
\end{aligned}$$

which completes the proof. □

3.4.2 Interpolation Application and Approximation

Let $b, c \in \ell^1(\mathbb{Z})$ with $c \geq 0$. We consider the operator $Q = W_{-1-c,b} + 2$ and denote by $\big(\lambda_j^-(Q)\big)_{j\geq 1}$ the sequence of negative eigenvalues $\lambda_j^-(Q)$ of the operator Q ordered by increasing modulus. If there are only finitely many negative eigenvalues, the sequence is continued with zeros. The map $(b, c) \mapsto \big(\lambda_j^-(Q)\big)_{j\geq 1}$, is not linear but by (3.8)

$$\sum_{j\geq 1} |\lambda_j^-(Q)|^{\frac{1}{2}} \leq 2L^{\mathrm{cl}}_{\frac{1}{2},1} \left(\|b\|_{\ell^1} + 2\,\|c\|_{\ell^1}\right)$$

and similarly for $b, c \in \ell^2(\mathbb{Z})$ with $c \geq 0$

$$\sum_{j\geq 1} |\lambda_j^-(Q)|^{\frac{3}{2}} \leq 2L^{\mathrm{cl}}_{\frac{3}{2},1} \left(\|b\|^2_{\ell^2} + 4\,\|c\|^2_{\ell^2}\right)$$

by (3.9). For $p_0 = 1, p_1 = 2$ consider decompositions $b = b_0 + b_1$ and $c = c_0 + c_1$ where $b_j, c_j \in \ell^{p_j}(\mathbb{Z})$ and $c_j \geq 0$. For $\theta \in (0, 1)$ we define the two operators

$$\begin{aligned}
(Q_0 u)(n) &= (-\theta - c_0(n-1))\, u(n-1) + (-\theta - c_0(n))\, u(n+1) + \big(b_0 + 2\theta\big)u(n)\,, \\
(Q_1 u)(n) &= (-1 + \theta - c_1(n-1))\, u(n-1) + (-1 + \theta - c_1(n))\, u(n+1) \\
&\quad + \big(b_1 + 2(1-\theta)\big)u(n)\,.
\end{aligned}$$

on $\ell^2(\mathbb{Z})$ such that $Q = Q_0 + Q_1$. The Min–Max principle (see e.g. [59, Theorem XIII.1]) states that for A denoting one of the operators Q, Q_0, Q_1 the negative eigenvalues can be computed as

$$\lambda_k^-(A) = \sup_{\varphi_1,\ldots,\varphi_{k-1}} \inf_{\substack{\psi \perp \varphi_1,\ldots,\varphi_{k-1} \\ \|\psi\|=1}} \langle A\psi, \psi\rangle \tag{3.10}$$

for $k \in \mathbb{N}$. Let $i, j \geq 1$ and choose $\varphi_1, \ldots, \varphi_{i-1}$ to be the first $i-1$ eigenfunctions of Q_0 and $\varphi_i, \ldots, \varphi_{i+j-2}$ the first $j-1$ eigenfunctions of Q_1. From (3.10) we can then conclude

that

$$\lambda^-_{i+j-1}(Q) \geq \inf_{\substack{\psi\perp\varphi_1,\dots,\varphi_{i+j-2}\\ \|\psi\|=1}} \langle Q\psi,\psi\rangle \geq \inf_{\substack{\psi\perp\varphi_1,\dots,\varphi_{i+j-2}\\ \|\psi\|=1}} \langle Q_0\psi,\psi\rangle + \inf_{\substack{\psi\perp\varphi_1,\dots,\varphi_{i+j-2}\\ \|\psi\|=1}} \langle Q_1\psi,\psi\rangle$$
$$\geq \lambda^-_i(Q_0) + \lambda^-_j(Q_1)\,.$$

We have seen that for all $i,j\in\mathbb{N}$

$$|\lambda^-_{i+j-1}(Q)| \leq |\lambda^-_i(Q_0)| + |\lambda^-_j(Q_1)|\,, \tag{3.11}$$

which is referred to as a Weyl inequality (see e.g. [10, Theorem 9.2.8]) and more generally as the Ky-Fan inequality (see e.g. [10, Section 11.1.3]) . To get an upper bound on $|\lambda^-_j(Q)|$ we construct the sequences ($N,j,r,s\in\mathbb{N}$)

$$\mu_j = \lambda^-_r(Q_0)\,, \qquad r = 1+\left[\frac{j}{1+N}\right],$$
$$\nu_j = \lambda^-_s(Q_1)\,, \qquad s = N\left[\frac{j}{1+N}\right] + \big(j \mod (1+N)\big),$$

where $[x]$ denotes the largest integer n such that $n\leq x$ for $x\in\mathbb{R}$. The numbers r,s were chosen such that $j=r+s-1$ and thus (3.11) implies that

$$|\lambda^-_j(Q)| \leq |\mu_j| + |\nu_j|\,.$$

Consequently we can compute that for the sequence $\big(\lambda^-_j(Q)\big)_{j\geq1}$ the inequality

$$K\left(\big(\lambda^-_j(Q)\big)_{j\geq1}, t, \frac{1}{2}, \frac{3}{2}\right) \leq \|(\mu_j)_{j\geq1}\|^{\frac12}_{\ell^{1/2}} + t\,\|(\nu_j)_{j\geq1}\|^{\frac32}_{\ell^{3/2}}$$
$$\leq (1+N)\sum_{i\geq1}|\lambda^-_i(Q_0)|^{\frac12} + t(1+N^{-1})\sum_{i\geq1}|\lambda^-_i(Q_1)|^{\frac32}$$

holds. Here we have used that an eigenvalue $\lambda^-_i(Q_0)$ is at most $(1+N)$ times repeated in the sequence $(\mu_j)_{j\geq1}$ and that every N-th eigenvalue $\lambda^-_{kN}(Q_1)$, $k\geq1$, is repeated once in

$(\nu_j)_{j\geq 1}$. We can now apply (3.8) and (3.9) to this inequality and obtain that

$$\begin{aligned} K\left(\left(\lambda_j^-(Q)\right)_{j\geq 1}, t, \frac{1}{2}, \frac{3}{2}\right) &\leq (1+N)2L^{\mathrm{cl}}_{\frac{1}{2},1}\theta^{-\frac{1}{2}}\left(\|b_0\|^1_{\ell^1} + 2\|c_0\|^1_{\ell^1}\right) \\ &\quad + t(1+N^{-1})2L^{\mathrm{cl}}_{\frac{3}{2},1}(1-\theta)^{-\frac{1}{2}}\left(\|b_1\|^2_{\ell^2} + 4\|c_1\|^2_{\ell^2}\right) \\ &= \frac{2(1+N)L^{\mathrm{cl}}_{\frac{1}{2},1}}{\theta^{\frac{1}{2}}}\left(\|b_0\|^1_{\ell^1} + Ct\|b_1\|^2_{\ell^2}\right) \\ &\quad + \frac{4(1+N)L^{\mathrm{cl}}_{\frac{1}{2},1}}{\theta^{\frac{1}{2}}}\left(\|c_0\|^1_{\ell^1} + 2Ct\|c_1\|^2_{\ell^2}\right), \end{aligned}$$

where

$$C := \frac{(1+N^{-1})\theta^{\frac{1}{2}}L^{\mathrm{cl}}_{\frac{3}{2},1}}{(1+N)(1-\theta)^{\frac{1}{2}}L^{\mathrm{cl}}_{\frac{1}{2},1}}.$$

Since the choice of $b_j, c_j \in \ell^{p_j}(\mathbb{Z})$ was arbitrary under the restriction that $c_j \geq 0$, we can take the infinum over all such sequences and arrive at

$$\begin{aligned} &K\left(\left(\lambda_j^-(Q)\right)_j, t, \frac{1}{2}, \frac{3}{2}\right) \\ &\leq \frac{2(1+N)L^{\mathrm{cl}}_{\frac{1}{2},1}}{\theta^{\frac{1}{2}}}\left(K\left(b, Ct, 1, 2\right) + 2\inf_{\substack{c=c_0+c_1 \\ c_j\geq 0, c_j\in\ell^{p_j}}}\left(\|c_0\|^1_{\ell^1} + 2Ct\|c_1\|^2_{\ell^2}\right)\right). \end{aligned}$$

We now want to prove that the second infinum can also be replaced by a K-function.

Lemma 3.4.2 *If c is a sequence such that $c \geq 0$ then*

$$\inf_{\substack{c=c_0+c_1 \\ c_j\in\ell^{p_j}}}\left(\|c_0\|^1_{\ell^1} + t\|c_1\|^2_{\ell^2}\right) = \inf_{\substack{c=c_0+c_1 \\ c_j\geq 0, c_j\in\ell^{p_j}}}\left(\|c_0\|^1_{\ell^1} + t\|c_1\|^2_{\ell^2}\right).$$

Proof As seen in the proof of Lemma 3.4.1 we note that

$$\inf_{\substack{c=c_0+c_1 \\ c_j\in\ell^{p_j}}}\left(\|c_0\|^1_{\ell^1} + t\|c_1\|^2_{\ell^2}\right) = \sum_{n\in\mathbb{Z}}|c(n)|\inf_{1=y_0+y_1}\left(|y_0| + t|u(n)||y_1|^2\right).$$

We first prove that for $s \geq 0$

$$\inf_{\substack{1=y_0+y_1\\ 0\leq y_j}} \left(|y_0| + s|y_1|^2\right) = \inf_{1=y_0+y_1} \left(|y_0| + s|y_1|^2\right). \tag{3.12}$$

Assume that $y_0 \geq 0$ and $y_1 \leq 0$ such that $1 = y_0 + y_1$. Then it must hold that $y_0 \geq 1$ and thus

$$|y_0| + s|y_1|^2 \geq 1 = |1| + s|0|^2.$$

Similarly, if $y_0 \leq 0$ and $y_1 \geq 0$ such that $1 = y_0 + y_1$, then $y_1 \geq 1$ and thus

$$|y_0| + s|y_1|^2 \geq s = |0| + s|1|^2.$$

As the case $y_0, y_1 \leq 0$ is not possible, we conclude that (3.12) is true. As a consequence it holds that

$$\inf_{c(n)=c_0(n)+c_1(n)} \left(|c_0(n)| + t|c_1(n)|^2\right) = \inf_{\substack{c(n)=c_0(n)+c_1(n)\\ 0\leq c_j(n)}} \left(|c_0(n)| + t|c_1(n)|^2\right)$$

and thus we obtain that

$$\begin{aligned}\inf_{\substack{c=c_0+c_1\\ c_j\in\ell^{p_j}}} \left(\|c_0\|_{\ell^1}^1 + t\,\|c_1\|_{\ell^2}^2\right) &= \sum_{n\in\mathbb{Z}} \inf_{\substack{c(n)=c_0(n)+c_1(n)\\ c_j(n)\geq 0}} \left(|c_0(n)| + t|c_1(n)|^2\right)\\ &= \inf_{\substack{c=c_0+c_1\\ c_j\geq 0,\, c_j\in\ell^{p_j}}} \left(\|c_0\|_{\ell^1}^1 + t\,\|c_1\|_{\ell^2}^2\right),\end{aligned}$$

which finishes the proof. □

Using Lemma 3.4.2 we now conclude that

$$K\left(\left(\lambda_j^-(Q)\right)_{j\geq 1}, t, \frac{1}{2}, \frac{3}{2}\right) \leq \frac{2(1+N)L^{\mathrm{cl}}_{\frac{1}{2},1}}{\theta^{\frac{1}{2}}}\big(K(b, Ct, 1, 2) + 2K(c, 2Ct, 1, 2)\big).$$

For $1/2 < \gamma < 3/2$ we apply the linear function $\Phi_{\eta,1}$ with $\eta = \gamma - \frac{1}{2}$ to this identity and use Lemma 3.4.1 to obtain that

$$\Theta\left(\eta, \frac{1}{2}, \frac{3}{2}\right) \sum_{j\geq 1} |\lambda_j^-(Q_0)|^\gamma \leq \frac{2(1+N)L^{\mathrm{cl}}_{\frac{1}{2},1}}{\theta^{\frac{1}{2}}} \Theta(\eta,1,2) C^\eta \left(\|b\|^{\gamma+\frac{1}{2}}_{\ell^{\gamma+\frac{1}{2}}} + 2^{\eta+1} \|c\|^{\gamma+\frac{1}{2}}_{\ell^{\gamma+\frac{1}{2}}} \right).$$

The constant in front of the $\ell^{\gamma+\frac{1}{2}}$ norms can be computed to be

$$\begin{aligned} &\frac{2(1+N)L^{\mathrm{cl}}_{\frac{1}{2},1}}{\theta^{\frac{1}{2}}} \Theta(\eta,1,2) C^\eta \\ &= 2^\eta (2L^{\mathrm{cl}}_{\frac{1}{2},1})^{1-\eta} (L^{\mathrm{cl}}_{\frac{3}{2},1})^\eta (1+N)^{1-\eta} (1+N^{-1})^\eta \theta^{-\frac{1}{2}(1-\eta)} (1-\theta)^{-\frac{\eta}{2}} \Theta(\eta,1,2)\,. \end{aligned}$$

We can still choose $N \in \mathbb{N}$ and $\theta \in (0,1)$ with respect to η such that this constant becomes minimal. A direct computation shows that the latter happens at $\theta = 1-\eta$. The definitions of μ_j and ν_j can be interchanged and consequently N and $1/N$ can change roles as well. We conclude that it is possible to consider N to be of the form k or $1/k$ with an integer k. Let $M(\eta)$ denote the minimum of

$$(1+N)^{1-\eta}(1+N^{-1})^\eta\,, N = \ldots, \frac{1}{3}, \frac{1}{2}, 2, 3 \ldots$$

then we have proved that

$$\sum_{j\geq 1} |\lambda_j^-(Q)|^\gamma \leq L^*_{\gamma,1} \left(\|b\|^{\gamma+\frac{1}{2}}_{\ell^{\gamma+\frac{1}{2}}} + 2^{\eta+1} \|a\|^{\gamma+\frac{1}{2}}_{\ell^{\gamma+\frac{1}{2}}} \right),$$

where

$$L^*_{\gamma,1} = 2^\eta (2L^{\mathrm{cl}}_{\frac{1}{2},1})^{1-\eta} (L^{\mathrm{cl}}_{\frac{3}{2},1})^\eta \frac{M(\eta)}{\sqrt{\eta^\eta (1-\eta)^{1-\eta}}} \frac{\Theta(\eta,1,2)}{\Theta(\eta, \frac{1}{2}, \frac{3}{2})}\,.$$

Choosing $c = -1 - a$ we can conclude that for the operator $W_{a,b}$ with $a \leq -1$ and with negative eigenvalues λ_j^- the spectral inequality

$$\sum_{j\geq 1} (|\lambda_j^-| - 2)^\gamma \leq L^*_{\gamma,1} \left(\sum_{n\in\mathbb{Z}} |b(n)|^{\gamma+\frac{1}{2}} + 2^{\gamma+\frac{1}{2}} \sum_{n\in\mathbb{Z}} |a(n)+1|^{\gamma+\frac{1}{2}} \right)$$

holds for all $1/2 < \gamma < 3/2$.

We can use this inequality to deduce a Lieb–Thirring inequality for the operator $H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$ with $V \in \mathcal{C}_c^\infty(\mathbb{R})$ and $V(x) \leq 0$ by means of the approximating Jacobi operators (3.5). Note that $a_k \leq -1$ if k is large enough. Denoting by $\mu_1, \dots, \mu_N$ the negative eigenvalues of H, we obtain that

$$\sum_{j\geq 1} |\mu_j|^{\gamma+\frac{1}{2}} \leq L^*_{\gamma,1} \left(c^{\gamma+\frac{1}{2}} + 2^{\gamma+\frac{1}{2}} d^{\gamma+\frac{1}{2}} \right) \int_{\mathbb{R}} |V(x)|^{\gamma+\frac{1}{2}} \, \mathrm{d}x \,.$$

Minimising the right-hand side with respect to $c \in [0,1]$ yields the Lieb–Thirring inequality

$$\sum_{j\geq 1} |\mu_j|^{\gamma+\frac{1}{2}} \leq L^{**}_{\gamma,1} \int_{\mathbb{R}} |V(x)|^{\gamma+\frac{1}{2}} \, \mathrm{d}x \,,$$

where

$$L^{**}_{\gamma,1} = 2^{\frac{1}{2}-\gamma} L^*_{\gamma,1} = (2L^{\mathrm{cl}}_{\frac{1}{2},1})^{\frac{3}{2}-\gamma} (L^{\mathrm{cl}}_{\frac{3}{2},1})^{\gamma-\frac{1}{2}} \frac{M(\gamma-\frac{1}{2})}{\sqrt{(\gamma-\frac{1}{2})^{\gamma-\frac{1}{2}} (\frac{3}{2}-\gamma)^{\frac{3}{2}-\gamma}}} \frac{\Theta(\gamma-\frac{1}{2},1,2)}{\Theta(\gamma-\frac{1}{2},\frac{1}{2},\frac{3}{2})} \,.$$

The assumptions $V \in \mathcal{C}_c^\infty(\mathbb{R})$ and $V(x) \leq 0$ can be relaxed to $V \in L^{\gamma+1/2}(\mathbb{R})$ by means of an approximation argument and the Min–Max principle. The same constant can be derived from the computations in [74], if the (then unknown) sharp value of $L_{1/2,1} = 2L^{\mathrm{cl}}_{1/2,1}$ is used. In this paper, more explicit expressions for the terms $\Theta(\gamma-\frac{1}{2},1,2)$ and $\Theta(\gamma-\frac{1}{2},\frac{1}{2},\frac{3}{2})$ can be found. The constants $L^{**}_{\gamma,1}$ are only sharp in the limiting cases $\gamma \to 1/2$ or $\gamma \to 3/2$.

The same results can be obtained by only considering Jacobi operators $W_{a,0}$ with vanishing potential $b \equiv 0$. To this end we use the symmetry argument of Section 3.3 to improve (3.8) and (3.9) to

$$\sum_{j\geq 1} (|\lambda_j^-| - 2)^{\frac{1}{2}} \leq 4L^{\mathrm{cl}}_{\frac{1}{2},1} \sum_{n\in\mathbb{Z}} |a(n)+1|$$

and

$$\sum_{j\geq 1} (|\lambda_j^-| - 2)^{\frac{3}{2}} \leq 4L^{\mathrm{cl}}_{\frac{3}{2},1} \sum_{n\in\mathbb{Z}} |a(n)+1|^2 \,,$$

respectively. The interpolation between these two inequalities can then be carried out in the exact same way as in the case of non-vanishing potentials and this yields again the constants $L^{**}_{\gamma,1}$ on the real line.

3.5 Conclusion

We summarise the conclusions that can be drawn from Chapters 2 and 3 with regards to the investigation of sharp Lieb–Thirring constants on the continuum through approximation by Jacobi operators.

As remarked in [42], the discrete case of a Jacobi operator differs in an important aspect from the case of a continuous differential operator $H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$. If the potential V in the definition of H is replaced by $\eta^2 V(\eta x)$, then the eigenvalues μ_j scale as $\eta^2\mu_j$. This implies that in a Lieb–Thirring inequality for H where the right-hand side is of the form $\int V(x)_-^{\gamma+1/2}\,\mathrm{d}x$, the left-hand side has to involve terms of the form $|\mu_j|^\gamma$. Such a relation does not hold for the Jacobi operator W and we have seen that the behaviour of the eigenvalues λ_j differs for large and small coupling. This led us to the left hand-side of (2.10) which has the required asymptotic behaviour for small eigenvalues as well as for large eigenvalues.

Using inequality (2.10) and approximation by discrete Schrödinger operators does not yield the sharp Lieb–Thirring constant on $L^2(\mathbb{R})$. This seems at first rather surprising as we have proved in Subsection 2.6.2 that the constant on the right-hand side of (2.10) is optimal. However, the inequality can be improved in different ways.

Firstly, our computations show that only the behaviour of (2.10) for small eigenvalues plays a role in the approximation procedure. As such it would be sufficient to consider spectral inequalities for the Jacobi operator where the left-hand side only contains terms of the form $(|\lambda_j| - 2)^\gamma$. Inequality (2.10) implies that (2.3) holds with the constant d_γ. No improvement is obtained here. Our results do not prove that the constant in (2.3) is optimal. In fact it is known that d_γ can be improved by a factor $\frac{\pi}{2\sqrt{3}}$ in the special case $1 \leq \gamma$ [63]. Better results for the Lieb–Thirring constants on the continuum can thus be expected by further improving the constant in inequality (2.3). This is not a contradiction to the sharpness of (2.10).

Secondly, the inequality (2.10) could be generalised from discrete Schrödinger operators to Jacobi operators with non-trivial off-diagonal entries. We have seen that at least in the case $\gamma = \frac{3}{2}$ this proves to be a fruitful approach. However, interpolation between (2.2) and (2.6), as undertaken in the previous section, did not lead to the sharp constant.

Finally, we note that the results of Section 3.2 and Section 3.3 show that (2.6) for Jacobi operators as well as for the special case of Jacobi operators with vanishing potentials is sufficient to obtain the sharp constant $L_{3/2,1}$ on $L^2(\mathbb{R})$. This is interesting, as we recall from

Subsection 2.6.1 that there exist explicit examples for both of these cases ($a \not\equiv -1, b \not\equiv 0$ and $a \not\equiv -1, b \equiv 0$) where inequality (2.6) is in fact an equality. Similarly, inequality (2.2), which yielded the sharp $L_{1/2,1}$, is not only optimal but there exists an optimiser, the delta potential, such that the inequality becomes an equality. In contrast, we are not aware of any optimisers for (2.10).

Chapter 4

Trace Formulae for Schrödinger Operators on Compact Intervals

The object of interest in this chapter is the Schrödinger operator

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\,, \quad x \in [0, b]\,, \tag{4.1}$$

where $b > 0$ is a positive constant and $V(x) \in \mathbb{R}^{m\times m}$ is a family of real, symmetric matrices. The domain of H is a subset of $L^2([0, b], \mathbb{C}^m)$. Introducing the Dirichlet boundary conditions $\psi(0) = \psi(b) = 0$ turns H into a self-adjoint operator (see e.g. [38, Theorem 4.2]). Similar to the well-known scalar case ($m = 1$), it can be shown that the spectrum of H consist solely of a countable number of eigenvalues μ_j, $j \in \mathbb{N}$, each of finite multiplicity $m_j \leq m$. These eigenvalues are discrete and can be arranged such that they tend to infinity, i.e. $\lim_{j\to\infty} \mu_j = \infty$. In the special case of a vanishing potential, $H_0 = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$, the eigenvalues can be calculated explicitly as $\mu_{j,0} = (j\pi/b)^2$ each with a multiplicity $m_j = m$. Our aim is to derive trace formulae for the negative eigenvalues of H.

We will prove Buslaev–Faddeev–Zakharov trace identities similar to (1.3). In contrast to the regularised trace formulae, we will also obtain identities for half-integer powers of the negative eigenvalues. In our approach we will closely follow [77].

In Section 4.1 we will define left-regular and right-regular solutions. These will be the analogue to the Jost solutions of a Schrödinger operator on the real line. We will then use a Wronskian-type matrix function to define the perturbation determinant. In Section 4.2 the high energy asymptotics of the perturbation determinant will be discussed. The main result of this chapter is Theorem 4.3.3 which introduces trace formulae of the Buslaev–Faddeev–

Zakharov type for the Schrödinger operator on a compact interval. The complete proof of these identities will be given in Section 4.3. In Section 4.4 we will show how the derived asymptotics can be used to prove regularised trace formulae.

4.1 Perturbation Determinant and Matrix-Valued Wronskian

The left-regular matrix-solution Ψ_- and the right-regular matrix-solution Ψ_+ satisfy the Dirichlet boundary conditions at only one endpoint and are defined as

$$\begin{cases} (H-\zeta^2)\,\Psi_-(x,\zeta)=0\,, \\ \Psi_-(0,\zeta)=0,\ \Psi_-'(0,\zeta)=\mathbb{I}\,, \end{cases} \qquad \begin{cases} (H-\zeta^2)\,\Psi_+(x,\zeta)=0\,, \\ \Psi_+(b,\zeta)=0,\ \Psi_+'(b,\zeta)=\mathbb{I}\,, \end{cases} \tag{4.2}$$

respectively. Here and in the remainder of this chapter, Ψ' refers to the derivative of Ψ with respect to $x\in[0,b]$. Similarly, the left-irregular and the right-irregular matrix-solutions, Θ_- and Θ_+, satisfy Neumann boundary conditions at one endpoint, i.e.

$$\begin{cases} (H-\zeta^2)\,\Theta_-(x,\zeta)=0\,, \\ \Theta_-(0,\zeta)=\mathbb{I},\ \Theta_-'(0,\zeta)=0\,, \end{cases} \qquad \begin{cases} (H-\zeta^2)\,\Theta_+(x,\zeta)=0\,, \\ \Theta_+(b,\zeta)=\mathbb{I},\ \Theta_+'(b,\zeta)=0\,. \end{cases}$$

Due to the different boundary values at zero, the two matrix-functions Ψ_- and Θ_- form a complete set of solutions of the matrix-valued differential equation $H-\zeta^2=0$ and consequently there exist matrices $A_1(\zeta)$, $A_2(\zeta)$ depending only on the parameter ζ such that

$$\Psi_+(x,\zeta)=\Psi_-(x,\zeta)A_1(\zeta)+\Theta_-(x,\zeta)A_2(\zeta)\,.$$

By evaluating this equation at the point $x=0$, we observe that $A_2(\zeta)=\Psi_+(0,\zeta)$.

Equivalently to (4.2), the right-regular solution Ψ_+ can be defined as a solution of the integral equation

$$\Psi_+(x,\zeta)=\frac{1}{\zeta}\sin\zeta(x-b)\mathbb{I}-\frac{1}{\zeta}\int_x^b \sin\zeta(x-y)V(y)\Psi_+(y,\zeta)\,\mathrm{d}y \tag{4.3}$$

and the following lemma can be shown to hold.

Lemma 4.1.1 *Let the potential satisfy the assumption $\|V(\cdot)\|\in L^1([0,b])$. Then the Volterra integral equation (4.3) has a unique solution which coincides with the solution*

of the second-order differential equation $-\Psi_+'' + (V - \zeta^2)\Psi_+ = 0$ *with boundary conditions* $\Psi_+(b,\zeta) = 0$, $\Psi_+'(b,\zeta) = \mathbb{I}$. *Furthermore* $\Psi_+(x,\zeta)$ *is an analytic function in the variable* $\zeta \neq 0$ *and satisfies* $\Psi_+(x,\zeta) = \Psi_+(x,-\zeta)$ *as well as* $\Psi_+(x,\zeta) = \overline{\Psi_+(x,-\overline{\zeta})}$.

Here and in the remainder of this chapter $\overline{A}$ denotes the component-wise complex conjugation of a matrix A. In terms of the adjoint A^* and the transpose A^{T}, the complex conjugation of A can be written as $\overline{A} = (A^{\mathrm{T}})^* = (A^*)^{\mathrm{T}}$.

Proof We follow the proofs of similar results in [23, 77]. Let $\Psi_0(x,\zeta) = \frac{1}{\zeta}\sin\zeta(x-b)\mathbb{I}$ and for $k \geq 0$ define recursively

$$\Psi_{k+1}(x,\zeta) = -\int_x^b \frac{1}{\zeta}\sin\zeta(x-y)V(y)\Psi_k(y,\zeta)\,\mathrm{d}y\,.$$

Clearly Ψ_0 is an analytic function of $\zeta \neq 0$ and by induction the same holds for any Ψ_k with $k \in \mathbb{N}$. Note that there exists a constant $C > 0$ such that $\|\zeta^{-1}\sin\zeta x\| \leq Cxe^{|\operatorname{Im}\zeta|x}$ for $x \geq 0$ and consequently

$$\|\Psi_0(x,\zeta)\| \leq C(b-x)\mathrm{e}^{|\operatorname{Im}\zeta|(b-x)} \leq D\mathrm{e}^{|\operatorname{Im}\zeta|(b-x)}\,.$$

This implies that

$$\begin{aligned}\|\Psi_1(x,\zeta)\| &\leq \int_x^b D\mathrm{e}^{|\operatorname{Im}\zeta|(y-x)}\,\|V(y)\|\,D\mathrm{e}^{|\operatorname{Im}\zeta|(b-y)}\,\mathrm{d}y\\ &= D^2\mathrm{e}^{|\operatorname{Im}\zeta|(b-x)}\int_x^b \|V(y)\|\,\mathrm{d}y\end{aligned}$$

and by induction we can show that

$$\|\Psi_k(x,\zeta)\| \leq D^{k+1}\mathrm{e}^{|\operatorname{Im}\zeta|(b-x)}\frac{1}{k!}\left(\int_x^b \|V(y)\|\,\mathrm{d}y\right)^k\,. \tag{4.4}$$

Thus the limit $\Psi_+(x,\zeta) = \lim_{n\to\infty}\sum_{k=0}^n \Psi_k(x,\zeta)$ exists uniformly for bounded ζ and x. A straightforward calculation shows that

$$\sum_{k=0}^n \Psi_k(x,\zeta) = \frac{1}{\zeta}\sin\zeta(x-b)\mathbb{I} - \int_x^b \frac{1}{\zeta}\sin\zeta(x-y)V(y)\sum_{k=0}^{n-1}\Psi_k(y,\zeta)\,\mathrm{d}y$$

and letting $n \to \infty$ proves that Ψ_+ solves the integral equation (4.3). As a locally uniform limit of analytic functions, Ψ_+ is itself analytic in $\zeta \neq 0$ and from (4.4) we can see that

$$\|\Psi_+(x,\zeta)\| \leq D\mathrm{e}^{|\operatorname{Im}\zeta|(b-x)} \exp\left(D\int_0^b \|V(y)\|\,\mathrm{d}y\right).$$

If $\widetilde{\Psi}_+$ is another bounded solution of (4.3) then the difference $\widetilde{\Psi}_+ - \Psi_+$ solves the corresponding homogeneous equation and an iteration procedure shows that the difference is bounded by (4.4) for all $k \in \mathbb{N}$. This allows us to conclude that $\widetilde{\Psi}_+ - \Psi_+ = 0$. An immediate consequence of this uniqueness is that $\Psi_+(x,\zeta) = \Psi_+(x,-\zeta)$. Taking the conjugate of $-\Psi_+''(x,\zeta) + (V(x) - \zeta^2)\Psi_+(x,\zeta) = 0$ and recalling that $V(x) \in \mathbb{R}^{m\times m}$, we observe that

$$-\overline{\Psi_+(x,\zeta)}'' + (V(x) - \overline{\zeta}^2)\overline{\Psi_+(x,\zeta)} = 0\,.$$

Since $\overline{\Psi_+(b,\zeta)} = 0$ and $\overline{\Psi_+(b,\zeta)'} = \mathbb{I}$, we can conclude that by the already discussed uniqueness $\overline{\Psi_+(x,\zeta)} = \Psi_+(x,-\overline{\zeta})$. □

In the scalar case, $m = 1$, the matrix $A_2(\zeta)$ can be identified with the Wronskian of Ψ_- and Ψ_+, which is defined as

$$W(\Psi_-,\Psi_+) = \Psi_-(x,\zeta)\Psi_+'(x,\zeta) - \Psi_-'(x,\zeta)\Psi_+(x,\zeta)\,. \tag{4.5}$$

By differentiating this function and using the defining differential equations (4.2) of Ψ_- and Ψ_+, it can be shown that the Wronskian is constant. Evaluating (4.5) at $x = 0$ yields the desired result, $A_2(\zeta) = -W(\Psi_-,\Psi_+)$. To establish a similar identity in the general, matrix-valued case, we first note that the Wronskian as defined in (4.5) is not a constant function for $m \geq 2$ due to the non-commutative nature of matrices. However, the adapted definition

$$W(\Psi_-,\Psi_+) = \Psi_-(x,-\overline{\zeta})^*\Psi_+'(x,\zeta) - \Psi_-'(x,-\overline{\zeta})^*\Psi_+(x,\zeta)$$

yields a constant function and it is easy to check that in the scalar case this expression coincides with the standard Wronskian. Evaluation at the point $x = 0$ shows that $A_2(\zeta) = -W(\Psi_-,\Psi_+)$. Furthermore it holds that the Green's function $G(x,y,\zeta)$ of the operator H

can be written as

$$G(x,y,\zeta) = \begin{cases} \Psi_-(x,\zeta)W(\Psi_+,\Psi_-)^{-1}\Psi_+(y,-\overline{\zeta})^*, & \text{if } x<y \\ -\Psi_+(x,\zeta)W(\Psi_-,\Psi_+)^{-1}\Psi_-(y,-\overline{\zeta})^*, & \text{if } x>y\,. \end{cases}$$

A proof of this result can be found in [36] (see also [54]) which allows us to state the following lemma.

Lemma 4.1.2 *The function* $\det A_2(\zeta)$ *vanishes at a complex* $\zeta \neq 0$ *if and only if* ζ^2 *is an eigenvalue of* H*. The multiplicity of a zero* ζ *is given by* $\dim\ker A_2(\zeta)$*, which is equal to the multiplicity of* ζ^2 *as an eigenvalue of* H*.*

Note that in the special case of a free Schrödinger operator, $H_0 = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$, the coefficient $A_2(\zeta)$ is exactly the matrix $-\frac{\sin\zeta b}{\zeta}\mathbb{I}$. To compare a general Schrödinger operator H to the unperturbed, free operator H_0, we define the perturbation determinant as

$$d(\zeta) := \det\left(\frac{-\zeta}{\sin\zeta b}A_2(\zeta)\right),$$

which is analytic on $\mathbb{C}\setminus\left\{\frac{n\pi}{b} : n\in\mathbb{Z}\right\}$. Note that in the literature the perturbation determinant is normally defined as $\det(\mathbb{I}+V(H_0-\zeta)^{-1})$ for ζ in the resolvent set of H_0. Without going into the connection of this definition to $d(\zeta)$, we want to emphasise that here we simply define the perturbation determinant to be $d(\zeta)$. By Lemma 4.1.2 the perturbation determinant has a zero of order m_j at the positive and negative square root of every eigenvalue μ_j and a pole of order m at every $\frac{n\pi}{b}$ with $n\in\mathbb{Z}$. Furthermore $d(\zeta) = d(-\zeta)$ and $d(\zeta) = \overline{d(-\overline{\zeta})}$.

4.2 High Energy Asymptotics

We are interested in the asymptotic representation of the perturbation determinant for $\zeta\to\infty$ and to this end first consider the asymptotic behaviour of Ψ_+.

Theorem 4.2.1 *Suppose that* $V\in\mathcal{C}^\infty([0,b],\mathbb{R}^{m\times m})$*. Then for any* $N\in\mathbb{N}$ *it holds that*

$$\Psi_+(x,\zeta) = \frac{\sin\zeta(x-b)}{\zeta}\sum_{k=0}^{N}\frac{B_k(x)}{(2\zeta)^k} + \frac{\cos\zeta(x-b)}{\zeta}\sum_{k=0}^{N}\frac{D_k(x)}{(2\zeta)^k} + R(x,\zeta,N)\,, \tag{4.6}$$

where $B_0(x) = \mathbb{I}$, $D_0(x) = 0$ *for all* $x \in [0, b]$ *and*

$$B_{k+1}(x) = -D_k'(x) - D_k'(b) - \int_x^b V(y) D_k(y)\, \mathrm{d}y\,, \tag{4.7}$$

$$D_{k+1}(x) = B_k'(x) - B_k'(b) + \int_x^b V(y) B_k(y)\, \mathrm{d}y\,, \tag{4.8}$$

for $k \in \mathbb{N}$. *For fixed* $c > 0$ *the remainder* R *satisfies the estimate*

$$\|R(x, \zeta, N)\| \leq C_N \frac{\mathrm{e}^{|\mathrm{Im}\,\zeta|(b-x)}}{|\zeta|^{N+2}}$$

for all $x \in [0, b]$ *and* $|\zeta| \geq c$. *The functions* $B_k : [0, b] \to \mathbb{R}^{m\times m}$ *are smooth with* $B_{k+1}(b) = -2D_k'(b)$ *for* $k \geq 0$ *and they vanish for odd indices,* $B_{2k+1} \equiv 0$ *for all* $k \geq 0$. *The functions* $D_k : [0, b] \to \mathbb{R}^{m\times m}$ *are smooth with* $D_k(b) = 0$ *for* $k \geq 0$ *and they vanish for even indices,* $D_{2k} \equiv 0$ *for all* $k \geq 0$.

Proof The smoothness of B_k and D_k follows by induction. Clearly $B_{k+1}(b) = -2D_k'(b)$, $D_k(b) = 0$ hold for $k \geq 0$ by definition. Since $D_0 \equiv 0$ we conclude from (4.7) that $B_1 \equiv 0$ and thus from (4.8) that $D_2 \equiv 0$. Proceeding by induction we can conclude that $B_{2k+1} \equiv 0 \equiv D_{2k}$ for all $k \geq 0$.

We now insert the expression (4.6) into the differential equation (4.2) for Ψ_+ and to this end compute that

$$\begin{aligned}\Psi_+'(x, \zeta) = {} & \frac{\sin \zeta(x-b)}{\zeta} \left(\sum_{k=0}^{N} \frac{B_k'(x)}{(2\zeta)^k} - \zeta \sum_{k=0}^{N} \frac{D_k(x)}{(2\zeta)^k} \right) \\ & + \frac{\cos \zeta(x-b)}{\zeta} \left(\zeta \sum_{k=0}^{N} \frac{B_k(x)}{(2\zeta)^k} + \sum_{k=0}^{N} \frac{D_k'(x)}{(2\zeta)^k} \right) + R'(x, \zeta, N)\,.\end{aligned} \tag{4.9}$$

Consequently the second derivative can be computed to be

$$\begin{aligned}\Psi_+''(x,\zeta) &= \frac{\sin\zeta(x-b)}{\zeta}\left(\sum_{k=0}^{N}\frac{B_k''(x)}{(2\zeta)^k} - \zeta^2\sum_{k=0}^{N}\frac{B_k(x)}{(2\zeta)^k} - 2\zeta\sum_{k=0}^{N}\frac{D_k'(x)}{(2\zeta)^k}\right)\\ &\quad + \frac{\cos\zeta(x-b)}{\zeta}\left(2\zeta\sum_{k=0}^{N}\frac{B_k'(x)}{(2\zeta)^k} - \zeta^2\sum_{k=0}^{N}\frac{D_k(x)}{(2\zeta)^k} + \sum_{k=0}^{N}\frac{D_k''(x)}{(2\zeta)^k}\right) + R''(x,\zeta,N)\\ &= \frac{\sin\zeta(x-b)}{\zeta}\left(\sum_{k=0}^{N}\frac{B_k''(x)}{(2\zeta)^k} - \frac{1}{4}\sum_{k=0}^{N}\frac{B_k(x)}{(2\zeta)^{k-2}} - \sum_{k=0}^{N}\frac{D_k'(x)}{(2\zeta)^{k-1}}\right)\\ &\quad + \frac{\cos\zeta(x-b)}{\zeta}\left(\sum_{k=0}^{N}\frac{B_k'(x)}{(2\zeta)^{k-1}} - \frac{1}{4}\sum_{k=0}^{N}\frac{D_k(x)}{(2\zeta)^{k-2}} + \sum_{k=0}^{N}\frac{D_k''(x)}{(2\zeta)^k}\right) + R''(x,\zeta,N)\,.\end{aligned}$$

Using that fact that $B_0'(x) = D_0'(x) = 0$ to change the indices in the summations of B_k' and D_k' we conclude that

$$\begin{aligned}\Psi_+''(x,\zeta) &= \frac{\sin\zeta(x-b)}{\zeta}\left(\sum_{k=0}^{N}\frac{B_k''(x)}{(2\zeta)^k} - \frac{1}{4}\sum_{k=0}^{N}\frac{B_k(x)}{(2\zeta)^{k-2}} - \sum_{k=0}^{N-1}\frac{D_{k+1}'(x)}{(2\zeta)^k}\right)\\ &\quad + \frac{\cos\zeta(x-b)}{\zeta}\left(\sum_{k=0}^{N-1}\frac{B_{k+1}'(x)}{(2\zeta)^k} - \frac{1}{4}\sum_{k=0}^{N}\frac{D_k(x)}{(2\zeta)^{k-2}} + \sum_{k=0}^{N}\frac{D_k''(x)}{(2\zeta)^k}\right) + R''(x,\zeta,N)\end{aligned}$$

holds. As Ψ_+ solves the differential equation (4.2), we now equate the above expression to

$$\begin{aligned}(V(x)-\zeta^2)\Psi_+(x,\zeta) &= \frac{\sin\zeta(x-b)}{\zeta}\left(\sum_{k=0}^{N}\frac{V(x)B_k(x)}{(2\zeta)^k} - \frac{1}{4}\sum_{k=0}^{N}\frac{B_k(x)}{(2\zeta)^{k-2}}\right)\\ &\quad + \frac{\cos\zeta(x-b)}{\zeta}\left(\sum_{k=0}^{N}\frac{V(x)D_k(x)}{(2\zeta)^k} - \frac{1}{4}\sum_{k=0}^{N}\frac{D_k(x)}{(2\zeta)^{k-2}}\right)\\ &\quad + \big(V(x)-\zeta^2\big)R(x,\zeta,N).\end{aligned}$$

To this end we first note that upon differentiation, (4.7) implies that

$$D_k''(x) - V(x)D_k(x) + B_{k+1}'(x) = 0$$

and (4.8) shows that

$$B_k''(x) - V(x)B_k(x) - D_{k+1}'(x) = 0\,.$$

Using these two identities, we observe that the differential equation for Ψ_+ implies that the remainder $R(x,\zeta,N)$ must satisfy

$$-R''(x,\zeta,N)+V(x)R(x,\zeta,N)=\zeta^2R(x,\zeta,N)+Q(x,\zeta,N)\,, \tag{4.10}$$

where the inhomogeneity Q is defined as

$$\begin{aligned}&Q(x,\zeta,N)\\&=\frac{1}{(2\zeta)^N}\left(\frac{\sin\zeta(x-b)}{\zeta}\big(V(x)B_N(x)-B_N''(x)\big)+\frac{\cos\zeta(x-b)}{\zeta}\big(V(x)D_N(x)-D_N''(x)\big)\right).\end{aligned}$$

We now investigate the boundary values of R. Since $\Psi_+(b,\zeta)=0$, we conclude from (4.6) that $R(x,\zeta,b)=0$. It also holds that $\Psi_+(b,\zeta)'=\mathbb{I}$ and thus we obtain from (4.9) that

$$\begin{aligned}0&=\sum_{k=0}^{N}\frac{B_k(b)}{(2\zeta)^k}+\frac{1}{\zeta}\sum_{k=0}^{N}\frac{D_k'(b)}{(2\zeta)^k}+R'(b,\zeta,N)-\mathbb{I}\\&=\sum_{k=1}^{N}\frac{B_k(b)}{(2\zeta)^k}+\frac{1}{\zeta}\sum_{k=0}^{N}\frac{D_k'(b)}{(2\zeta)^k}+R'(b,\zeta,N)\\&=\sum_{k=0}^{N-1}\frac{B_{k+1}(b)}{(2\zeta)^{k+1}}+2\sum_{k=0}^{N}\frac{D_k'(b)}{(2\zeta)^{k+1}}+R'(b,\zeta,N)\,.\end{aligned}$$

Together with the fact that $B_{k+1}(b)=-2D_k'(b)$ we thus have

$$0=2\frac{D_N'(b)}{(2\zeta)^{N+1}}+R'(b,\zeta,N).$$

We can conclude that $R(x,\zeta,N)$ satisfies the differential equation (4.10) and the boundary conditions

$$R(b,\zeta,N)=0\,,\quad R'(b,\zeta,N)=-2\frac{D_N'(b)}{(2\zeta)^{N+1}}\,. \tag{4.11}$$

The differential equation (4.10) is of the same form as (4.2) with the exception of the boundary conditions and the inhomogeneity $Q(x,\zeta,N)$. To solve it, we first rewrite it as

an integral equation. We consider the function

$$P(x,\zeta,N) = \frac{1}{\zeta}\int_x^b \sin\zeta(x-y)Q(y,\zeta,N)\,\mathrm{d}y\,,$$

which is chosen such that

$$P'(x,\zeta,N) = \int_x^b \cos\zeta(x-y)Q(y,\zeta,N)\,\mathrm{d}y$$

and which thus satisfies

$$\begin{aligned} P''(x,\zeta,N) &= -Q(x,\zeta,N) - \zeta\int_x^b \sin\zeta(x-y)Q(y,\zeta,N)\,\mathrm{d}y \\ &= -Q(x,\zeta,N) - \zeta^2 P(x,\zeta,N)\,. \end{aligned}$$

As a consequence we obtain that the differential equation (4.10) with boundary conditions (4.11) is equivalent to the integral equation

$$\begin{aligned} &R(x,\zeta,N) \\ &= P(x,\zeta,N) + \frac{\sin\zeta(x-b)}{\zeta}R'(b,\zeta,N) - \frac{1}{\zeta}\int_x^b \sin\zeta(x-y)V(y)R(y,\zeta,N)\,\mathrm{d}y\,. \end{aligned} \tag{4.12}$$

This integral equation can be solved by a similar method as used in the proof of Lemma 4.1.1. First we note that for $x \geq 0$

$$|\sin\zeta x| \leq \mathrm{e}^{|\mathrm{Im}\,\zeta|x}, \quad |\cos\zeta x| \leq \mathrm{e}^{|\mathrm{Im}\,\zeta|x}\,,$$

and consequently there exists a constant $C_1 > 0$ such that for all $|\zeta| \geq c$

$$\|Q(x,\zeta,N)\| \leq C_1\frac{\mathrm{e}^{|\mathrm{Im}\,\zeta|(b-x)}}{|\zeta|^{N+1}}\,.$$

This allows us to conclude that the function P can be bounded by a similar expression

$$\|P(x,\zeta,N)\| \leq \frac{C_1}{|\zeta|^{N+2}}\int_x^b \mathrm{e}^{|\mathrm{Im}\,\zeta|(y-x)}\mathrm{e}^{|\mathrm{Im}\,\zeta|(b-y)}\,\mathrm{d}y \leq C_2\frac{\mathrm{e}^{|\mathrm{Im}\,\zeta|(b-x)}}{|\zeta|^{N+2}}\,.$$

Furthermore we observe that the smoothness of D_k and the compactness of $[0, b]$ imply that

$$\left\| \frac{\sin \zeta(x-b)}{\zeta} R'(b, \zeta, N) \right\| \leq C_3 \frac{\mathrm{e}^{|\operatorname{Im} \zeta|(b-x)}}{|\zeta|^{N+2}}$$

for $|\zeta| \geq c$. We now define the matrix function $R_0(x, \zeta, N)$ as

$$R_0(x, \zeta, N) = P(x, \zeta, N) + \frac{\sin \zeta(x-b)}{\zeta} R'(b, \zeta, N)$$

and define recursively for $k \geq 0$

$$R_{k+1}(x, \zeta, N) = -\frac{1}{\zeta} \int_x^b \sin \zeta(x-y) V(y) R_k(y, \zeta, N) \, \mathrm{d}y \, .$$

An induction argument shows that all the matrix functions $R_k(x, \zeta, N)$ are smooth in x and analytic in $\zeta \neq 0$. From the already established bounds we can conclude that

$$\|R_0(x, \zeta, N)\| \leq C_5 \mathrm{e}^{|\operatorname{Im} \zeta|(b-x)}$$

for $|\zeta| \geq c$ and using an induction argument we can show that

$$\|R_k(x, \zeta, N)\| \leq C_5^{k+1} \mathrm{e}^{|\operatorname{Im} \zeta|} \frac{1}{n!} \left(\int_x^b \|V(y)\| \, \mathrm{d}y \right)^k .$$

Thus the limit $R(x, \zeta, N) = \lim_{n \to \infty} \sum_{k=0}^n R_k(x, \zeta, N)$ exists uniformly for bounded $|\zeta| \geq c$ and $x \in [0, b]$. Since $c > 0$ can be chosen to be arbitrarily small, $R(x, \zeta, N)$ is analytic in $\zeta \neq 0$ as a locally uniform limit of analytic functions. We compute that

$$\begin{aligned} &\sum_{k=0}^n R_k(x, \zeta, N) \\ &= P(x, \zeta, N) + \frac{\sin \zeta(x-b)}{\zeta} R'(b, \zeta, N) - \frac{1}{\zeta} \int_x^b \sin \zeta(x-y) V(y) \sum_{k=0}^{n-1} R_k(y, \zeta, N) \, \mathrm{d}y \end{aligned}$$

and letting $n \to \infty$ proves that the so-defined $R(x, \zeta, N)$ solves the integral equation

(4.12). Furthermore the bound

$$\|R(x,\zeta,N)\| \leq C_5 \mathrm{e}^{|\mathrm{Im}\,\zeta|(b-x)} \exp\left(C_5 \int_0^b \|V(y)\|\ \mathrm{d}y\right) \leq C_6 \mathrm{e}^{|\mathrm{Im}\,\zeta|(b-x)}$$

holds for all $|\zeta| \geq c$. We can now insert this bound into the integral equation (4.12) and can conclude that the better upper bound $\|R(x,\zeta,N)\| \leq C_7 \mathrm{e}^{|\mathrm{Im}\,\zeta|(b-x)}/|\zeta|$ holds. We can insert this bound again into (4.12) and continue in this manner until we arrive at the desired result $\|R(x,\zeta,N\| \leq C_8 \mathrm{e}^{|\mathrm{Im}\,\zeta|(b-x)}/|\zeta|^{N+2}$. The uniqueness of the solution $R(x,\zeta,N)$ follows from a similar argument as in the proof of Lemma 4.1.1. □

A similar expansion can be computed for the matrix function Ψ_-. To this end we consider the new Schrödinger operator

$$\widehat{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(b-x)\,, \quad x \in [0,b]\,,$$

with Dirichlet boundary conditions. Then, if ψ is an eigenfunction of H to the eigenvalue μ, the vector function $\widehat{\psi}(x) = \psi(b-x)$ satisfies

$$\begin{aligned}(\widehat{H}\widehat{\psi})(x) &= -\widehat{\psi}''(x) + V(b-x)\widehat{\psi}(x) = -\psi''(b-x) + V(b-x)\psi(b-x) = \mu\psi(b-x) \\ &= \mu\widehat{\psi}(x)\,.\end{aligned}$$

Since $\widehat{\psi}$ clearly also satisfies the Dirichlet boundary conditions, we can conclude that the spectrum of $\widehat{H}$ is the same as the spectrum of H. Furthermore, we can conclude that the regular matrix-solutions $\widehat{\Psi}_+$ and $\widehat{\Psi}_-$ of $\widehat{H}$ are given by $\widehat{\Psi}_+(x) = \Psi_-(b-x)$ and $\widehat{\Psi}_-(x) = \Psi_+(b-x)$. The established results can now be now applied to $\widehat{\Psi}_+$ and thus we obtain that

$$\Psi_-(x,\zeta) = \frac{\sin\zeta x}{\zeta} \sum_{k=0}^{N} \frac{B_k(b-x)}{(2\zeta)^k} + \frac{\cos\zeta x}{\zeta} \sum_{k=0}^{N} \frac{D_k(b-x)}{(2\zeta)^k} + R(b-x,\zeta,N)\,.$$

The matrix functions B_k and D_k can be computed recursively from (4.7) and (4.8). The first three non-vanishing functions are given by

$$
\begin{aligned}
B_0(x) &= \mathbb{I}\,,\\
D_1(x) &= \int_x^b V(y)\,\mathrm{d}y\,,\\
B_2(x) &= V(x) + V(b) - \int_x^b \int_y^b V(y)V(z)\,\mathrm{d}z\,\mathrm{d}y\,,\\
D_3(x) &= V'(x) - V'(b) + V(x)\int_x^b V(y)\,\mathrm{d}y + \int_x^b V(y)^2\,\mathrm{d}y + \int_x^b V(y)\,\mathrm{d}y V(b)\,\mathrm{d}y\\
&\quad - \int_x^b \int_y^b \int_z^b V(y)V(z)V(w)\,\mathrm{d}w\,\mathrm{d}\,\mathrm{d}z\,\mathrm{d}y\,.
\end{aligned}
$$

Note that, with the exception of the scalar $m = 1$ case, the non-commutative nature of matrices does not allow us to further simplify the integrals of $V(y)V(z)$ and $V(y)V(z)V(w)$.

With the aim of computing the asymptotic expansion of $\log d(\zeta)$, we note that Theorem 4.2.1 with $x = 0$ shows that

$$
\frac{-\zeta}{\sin\zeta b}\Psi_+(0,\zeta) = \sum_{k=0}^{N}\frac{B_k(0)}{(2\zeta)^k} - \frac{\cos\zeta b}{\sin\zeta b}\sum_{k=0}^{N}\frac{D_k(0)}{(2\zeta)^k} + Q(\zeta,N) \tag{4.13}
$$

for all $\zeta \in \mathbb{C}\setminus\{\pm(j\pi)/b : j \in \mathbb{N}\cup\{0\}\}$, i.e. for all ζ which are no roots of the eigenvalues of $H_0 = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$. Here, the remainder $Q(\zeta, N)$ is defined as

$$
Q(\zeta,N) = -\frac{\zeta}{\sin\zeta b}R(0,\zeta,N)\,.
$$

For fixed $\varepsilon > 0$, Theorem 4.2.1 shows that $Q(\zeta, N)$ satisfies

$$
\|Q(\zeta,N)\| \leq C\frac{1}{|\zeta|^{N+1}}
$$

for all $\zeta \in \mathbb{C}$ such that $|\zeta \pm (j\pi)/b| \geq \varepsilon$ for all $j \in \mathbb{N}\cup\{0\}$. For convenience we introduce the notation $\Omega_\varepsilon = \{\zeta \in \mathbb{C} : |\zeta \pm (j\pi)/b| \geq \varepsilon \text{ for all } j \in \mathbb{N}\cup\{0\}\}$. We list the first three

non-zero matrices $B_k(0)$ and $D_k(0)$ in the expansion (4.13) as

$$\begin{aligned}
B_0(0) &= \mathbb{I}\,,\\
D_1(0) &= \int_0^b V(y)\,\mathrm{d}y\,,\\
B_2(0) &= V(0) + V(b) - \int_0^b \int_y^b V(y)V(z)\,\mathrm{d}z\,\mathrm{d}y\,,\\
D_3(0) &= V(0)' - V'(b) + V(0)\int_0^b V(y)\,\mathrm{d}y + \int_0^b V(y)\,\mathrm{d}y V(b) + \int_0^b V(y)^2\,\mathrm{d}y\\
&\quad - \int_0^b \int_y^b \int_z^b V(y)V(x)V(w)\,\mathrm{d}w\,\mathrm{d}z\,\mathrm{d}y\,.
\end{aligned}$$

Since it holds that

$$\left|\frac{\cos\zeta b}{\sin\zeta b}\right| \leq C$$

for all $\zeta \in \Omega_\varepsilon$ and since $B_0 \equiv \mathbb{I}$, $D_0 \equiv 0$, the matrix $\frac{-\zeta}{\sin\zeta b}\Psi_+(0,\zeta)$ is invertible for sufficiently large $|\zeta|$ in Ω_ε. Thus its logarithm is well-defined and Liouville's formula states that

$$\log d(\zeta) = \log\det\left(\frac{-\zeta}{\sin\zeta b}\Psi_+(0,\zeta)\right) = \operatorname{tr}\log\left(\frac{-\zeta}{\sin\zeta b}\Psi_+(0,\zeta)\right)\,.$$

This allows us to compute the asymptotic expansion of $\log d(\zeta)$ via the well known Taylor series of $\log(1+z)$.

Theorem 4.2.2 *Suppose that $V \in \mathcal{C}^\infty([0,b],\mathbb{R}^{m\times m})$ and let $\varepsilon > 0$. Then there exist coefficients $\ell_{i,j} \in \mathbb{R}$ such that for any $N \in \mathbb{N}$*

$$\log d(\zeta) = \sum_{j=1}^{N} \frac{1}{(2\zeta)^j}\left(\sum_{i=0}^{j} \ell_{i,j}\left(\frac{\cos\zeta b}{\sin\zeta b}\right)^i\right) + r(\zeta,N),$$

where the remainder satisfies the estimate

$$|r(\zeta,N)| \leq C_N \frac{1}{|\zeta|^{N+1}}$$

for all $\zeta \in \Omega_\varepsilon$. It holds that $\ell_{i,j} = 0$ if either $i \in 2\mathbb{N}-1, j \in 2\mathbb{N}$ or if $i \in 2\mathbb{N}\cup\{0\}, j \in$

$2\mathbb{N}+1$.

The last assertion is an immediate consequence of $B_{2k+1} \equiv 0 \equiv D_{2k}$ for $k \geq 0$ and reflects the fact that $d(\zeta) = d(-\zeta)$. The explicit computations of $\ell_{i,j}$ are straightforward but rather lengthy. We shall give the first few terms for later reference as

$$\begin{aligned}\log d(\zeta) &= -\frac{1}{2\zeta}\frac{\cos\zeta b}{\sin\zeta b}\mathrm{tr}D_1(0) + \frac{1}{(2\zeta)^2}\mathrm{tr}B_2(0) - \frac{1}{(2\zeta)^2}\left(\frac{\cos\zeta b}{\sin\zeta b}\right)^2\frac{1}{2}\mathrm{tr}D_1(0)^2 + r(\zeta,2)\\ &= -\frac{1}{2\zeta}\frac{\cos\zeta b}{\sin\zeta b}\int_0^b \mathrm{tr}V(y)\,\mathrm{d}y + \frac{1}{(2\zeta)^2}\left(\mathrm{tr}V(0) + \mathrm{tr}V(b) - \frac{1}{2}\mathrm{tr}\left(\int_0^b V(y)\,\mathrm{d}y\right)^2\right)\\ &\quad - \frac{1}{(2\zeta)^2}\left(\frac{\cos\zeta b}{\sin\zeta b}\right)^2\frac{1}{2}\mathrm{tr}\left(\int_0^b V(y)\,\mathrm{d}y\right)^2 + r(\zeta,2)\,.\end{aligned}$$

With regards to low-energy asymptotics, we aim to show that $\zeta\log d(\zeta)$ vanishes as $\zeta\to 0$ with $\varepsilon \leq \arg\zeta \leq \pi-\varepsilon$. Following the computations in [77], we can show that $d(\zeta)$ is continuous at 0. Unlike the case of a Schrödinger operator on the real line, $d(0)=0$ is equivalent to 0 being an eigenvalue of the operator. This eigenvalue can be most of order m and consequently $d(\zeta)$ can only have a zero of order m at $\zeta=0$. In particular, we can conclude that $\lim_{\zeta\to 0}\zeta\log d(\zeta) = 0$.

4.3 Trace Formulae of the Buslaev–Faddeev–Zakharov Type

In this section we aim to prove trace formulae for the negative eigenvalues of H. Since $\lim_{j\to\infty}\mu_j = \infty$, only finitely many negative eigenvalues $\mu_1,\dots,\mu_N$ exist with multiplicities $m_1,\dots,m_N$. Let $\alpha_j \in [0,\infty)$ such that $(\mathrm{i}\alpha_j)^2 = \mu_j$ for $j=1,\dots,N$. In the sector $\Lambda_\varepsilon = \{\zeta\in\mathbb{C}:\ \varepsilon\leq\arg\zeta\leq\pi-\varepsilon\}$ it holds for $|\zeta|\geq c>0$ that

$$\left|\frac{\cos\zeta b}{\mathrm{i}\sin\zeta b}+1\right| = \left|\frac{2\mathrm{e}^{2\mathrm{i}\zeta b}}{1-\mathrm{e}^{2\mathrm{i}\zeta b}}\right| \leq C\mathrm{e}^{-\mathrm{Im}\,\zeta b}\,.$$

Thus $\cos\zeta b/\sin\zeta b$ converges to the complex number $1/\mathrm{i}$ as $|\zeta|\to\infty$ in Λ_ε faster than any power of $1/\zeta$. We conclude that we can replace $\cos\zeta b/\sin\zeta b$ in (4.13) with the complex number $1/\mathrm{i}$ without changing the properties of the remainder, such that

$$-\frac{\zeta}{\sin\zeta b}\Psi_+(0,\zeta) = \sum_{k=0}^N\frac{B_k(0)}{(2\zeta)^k} - \frac{1}{\mathrm{i}}\sum_{k=0}^N\frac{D_k(0)}{(2\zeta)^k} + Q(\zeta,N)\,.$$

Since B_k vanishes for odd k and D_k vanishes for even k we can rewrite the asymptotic expansion using only one power series. For convenience we write the expansion with respect to powers of $1/(2\mathrm{i}\zeta)$ instead of $1/(2\zeta)$. To this end we set $E_{2k}(x) = (-1)^k B_{2k}(x)$ and $E_{2k+1}(x) = -(-1)^k D_{2k+1}(x)$ for $k \geq 0$. Using (4.7) we conclude that

$$\begin{aligned} E_{2k}(x) &= (-1)^k B_{2k}(x) \\ &= -(-1)^k D'_{2k-1}(x) - (-1)^k D'_{2k-1}(b) - \int_x^b V(y)(-1)^k D_{2k-1}(y)\,\mathrm{d}y \\ &= -E'_{2k-1}(x) - E'_{2k-1}(b) - \int_x^b V(y) E_{2k-1}(y)\,\mathrm{d}y \end{aligned}$$

and using (4.8) that

$$\begin{aligned} E_{2k+1}(x) &= -(-1)^k D_{2k+1}(x) \\ &= -(-1)^k B'_{2k}(x) + (-1)^k B'_{2k}(b) - \int_x^b V(y)(-1)^k B_{2k}(y)\,\mathrm{d}y \\ &= -E'_{2k}(x) + E'_{2k}(b) - \int_x^b V(y) E_{2k}(y)\,\mathrm{d}y\,. \end{aligned}$$

The results are summarised in the following Corollary.

Corollary 4.3.1 *Suppose that $V \in \mathcal{C}^\infty([0,b], \mathbb{R}^{m\times m})$. Then for any $N \in \mathbb{N}$ and $\varepsilon > 0$ it holds that*

$$-\frac{\zeta}{\sin \zeta b}\Psi_+(0,\zeta) = \sum_{k=0}^{N} \frac{E_k(0)}{(2\mathrm{i}\zeta)^k} + Q(\zeta, N)$$

for all $\zeta \in \Lambda_\varepsilon$, where $E_0(x) = \mathbb{I}$ for all $x \in [0,b]$ and

$$E_{k+1}(x) = -E'_k(x) + (-1)^k E'_k(b) - \int_x^b V(y) E_k(y)\,\mathrm{d}y$$

for $k \in \mathbb{N}$. The remainder Q satisfies the estimate

$$\|Q(\zeta, N)\| \leq C_N \frac{1}{|\zeta|^{N+1}}$$

for all $\zeta \in \Lambda_\varepsilon$.

For convenience, we write down the first few matrices $E_k(0)$ as

$$\begin{aligned}
E_0(0) &= \mathbb{I}\,,\\
E_1(0) &= -\int_0^b V(y)\,\mathrm{d}y\,,\\
E_2(0) &= -V(0) - V(b) + \int_0^b \int_y^b V(y)V(z)\,\mathrm{d}z\,\mathrm{d}y\,,\\
E_3(0) &= V'(0) - V'(b) + V(0)\int_0^b V(y)\,\mathrm{d}y + \int_0^b V(y)\,\mathrm{d}yV(b) + \int_0^b V(y)^2\,\mathrm{d}y\\
&\quad - \int_0^b \int_y^b \int_z^b V(y)V(x)V(w)\,\mathrm{d}w\,\mathrm{d}z\,\mathrm{d}y\,.
\end{aligned}$$

We can now investigate the asymptotic expansion of $\log d(\zeta)$ in Λ_ε using Liouville's formula. The results are less complicated than the expressions found in Theorem 4.2.2.

Corollary 4.3.2 *Suppose that $V \in \mathcal{C}^\infty([0,b],\mathbb{R}^{m\times m})$. Then for any $N \in \mathbb{N}$ and $\varepsilon > 0$ there exist coefficients $\ell_k \in \mathbb{R}$ such that*

$$\log d(\zeta) = \sum_{k=1}^{N} \frac{\ell_k}{(2\mathrm{i}\zeta)^k} + r(\zeta, N)\,.$$

The remainder satisfies the estimate

$$|r(\zeta,N)| \le C_N \frac{1}{|\zeta|^{N+1}}$$

for all $\zeta \in \Lambda_\varepsilon$.

The first three coefficients can be computed to be

$$\begin{aligned}
\ell_1 &= -\int_0^b \mathrm{tr}V(x)\,\mathrm{d}x\,,\\
\ell_2 &= -\mathrm{tr}V(0) - \mathrm{tr}V(b)\,,\\
\ell_3 &= \mathrm{tr}V'(0) - \mathrm{tr}V'(b) + \int_0^b \mathrm{tr}V(x)^2\,\mathrm{d}x\,.
\end{aligned}$$

We recall that $d(\zeta) = d(-\zeta)$ and thus can conclude that

$$\log d(\zeta) = \log d(-\zeta) = \sum_{k=1}^{\infty} \frac{\ell_k}{(-2\mathrm{i}\zeta)^k} = \sum_{k=1}^{\infty} \frac{(-1)^k \ell_k}{(2\mathrm{i}\zeta)^k}$$

as $|\zeta| \to \infty$ in $\Lambda_\varepsilon' = -\Lambda_\varepsilon = \{\zeta \in \mathbb{C} : -\pi + \varepsilon \leq \arg \zeta \leq -\varepsilon\}$.

We now use contour integration to establish trace formulae of the Buslaev–Faddeev–Zakharov type. Let $\gamma_{R,\varepsilon}$ be the counter-clockwise contour (see Figure 4.1) which consists of the arc

$$\gamma_{R,\varepsilon}^1 = \{\zeta \in \mathbb{C} : |\zeta| = R, \varepsilon \leq \arg \zeta \leq \pi - \varepsilon\}$$

and the two lines

$$\gamma_{R,\varepsilon}^2 = \{\zeta \in \mathbb{C} : |\zeta| \leq R, \arg \zeta = \pi - \varepsilon\},$$
$$\gamma_{R,\varepsilon}^3 = \{\zeta \in \mathbb{C} : |\zeta| \leq R, \arg \zeta = \varepsilon\}.$$

Let k be a fixed integer with $k \geq 1$. An application of the residue theorem shows that

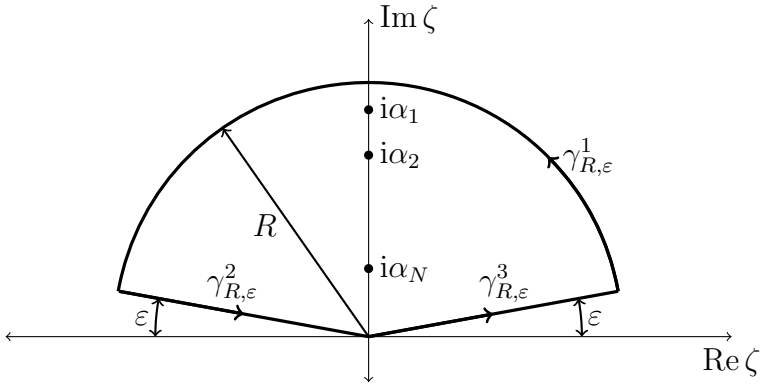


Figure 4.1: The contour $\gamma_{R,\varepsilon} = \gamma_{R,\varepsilon}^1 \oplus \gamma_{R,\varepsilon}^2 \oplus \gamma_{R,\varepsilon}^3$

$$\int_{\gamma_{R,\varepsilon}} \zeta^k \left(\frac{\frac{\mathrm{d}}{\mathrm{d}\zeta} d(\zeta)}{d(\zeta)} + \sum_{j=1}^{k-1} \frac{j\ell_j}{(2\mathrm{i})^j \zeta^{j+1}} \right) \mathrm{d}\zeta = 2\pi \mathrm{i}^{k+1} \sum_{j=1}^{N} m_j \alpha_j^k \,.$$

We now consider the integral over the arc $\gamma^1_{R,\varepsilon}$ and use integration by parts to compute that

$$\begin{aligned}&\int_{\gamma^1_{R,\varepsilon}} \zeta^k \left(\frac{\frac{\mathrm{d}}{\mathrm{d}\zeta} d(\zeta)}{d(\zeta)} + \sum_{j=1}^{k-1} \frac{j\ell_j}{(2\mathrm{i})^j \zeta^{j+1}} \right) \mathrm{d}\zeta \\ &= \zeta^k \left(\log d(\zeta) - \sum_{j=1}^{k-1} \frac{\ell_j}{(2\mathrm{i}\zeta)^j} \right) \Bigg|_{\zeta=R\mathrm{e}^{\mathrm{i}\varepsilon}}^{\zeta=-R\mathrm{e}^{-\mathrm{i}\varepsilon}} - k \int_{\gamma^1_{R,\varepsilon}} \zeta^{k-1} \left(\log d(\zeta) - \sum_{j=1}^{k-1} \frac{\ell_j}{(2\mathrm{i}\zeta)^j} \right) \mathrm{d}\zeta \,.\end{aligned}$$

We first investigate the boundary term and note that by Corollary 4.3.2

$$\lim_{R\to\infty} \zeta^k \left(\log d(\zeta) - \sum_{j=1}^{k-1} \frac{\ell_j}{(2\mathrm{i}\zeta)^j} \right) \Bigg|_{\zeta=R\mathrm{e}^{\mathrm{i}\varepsilon}}^{\zeta=-R\mathrm{e}^{-\mathrm{i}\varepsilon}} = \lim_{R\to\infty} \zeta^k \left(\frac{\ell_k}{(2\mathrm{i}\zeta)^k} + r(\zeta,k) \right) \Bigg|_{\zeta=R\mathrm{e}^{\mathrm{i}\varepsilon}}^{\zeta=-R\mathrm{e}^{-\mathrm{i}\varepsilon}} = 0 \,.$$

Using again the asymptotic behaviour derived in Corollary 4.3.2, the remaining integral over the arc $\gamma^1_{R,\varepsilon}$ can be computed to be

$$\begin{aligned}&\lim_{R\to\infty} \int_{\gamma^1_{R,\varepsilon}} \zeta^{k-1} \left(\log d(\zeta) - \sum_{j=1}^{k-1} \frac{\ell_j}{(2\mathrm{i}\zeta)^j} \right) \mathrm{d}\zeta \\ &\quad = \mathrm{i} \lim_{R\to\infty} \int_{\varepsilon}^{\pi-\varepsilon} R^k \mathrm{e}^{\mathrm{i}\theta k} \left(\frac{\ell_k}{R^k \mathrm{e}^{\mathrm{i}\theta k} (2\mathrm{i})^k} + r(R\mathrm{e}^{\mathrm{i}\theta}, k) \right) \mathrm{d}\theta \\ &\quad = (\pi - 2\varepsilon) \frac{\ell_k}{2^k \mathrm{i}^{k-1}} \,.\end{aligned}$$

In a similar way, we can apply integration by parts to the integral along $\gamma^2_{R,\varepsilon} \oplus \gamma^3_{R,\varepsilon}$ and again the boundary terms vanish by Corollary 4.3.2 as $R \to \infty$ such that

$$\begin{aligned}&\lim_{R\to\infty} \int_{\gamma^2_{R,\varepsilon} \oplus \gamma^3_{R,\varepsilon}} \zeta^k \left(\log d(\zeta) - \sum_{j=1}^{k-1} \frac{\ell_j}{(2\mathrm{i}\zeta)^j} \right) \mathrm{d}\zeta \\ &= -k \lim_{R\to\infty} \int_{\gamma^2_{R,\varepsilon} \oplus \gamma^3_{R,\varepsilon}} \zeta^{k-1} \left(\log d(\zeta) - \sum_{j=1}^{k-1} \frac{\ell_j}{(2\mathrm{i}\zeta)^j} \right) \mathrm{d}\zeta \,.\end{aligned}$$

Note that, in order to make the computations rigorous, we also need to introduce a small semicircle that connects $\gamma^2_{R,\varepsilon}$ and $\gamma^3_{R,\varepsilon}$ and avoids the point $\zeta = 0$. The integral over this arc can again be computed using integration by parts. As d can only have a zero of finite multiplicity m at $\zeta = 0$, we see that the integral vanishes as the radius of the semicircle tends to 0.

To shorten notation, we introduce the definition $\gamma_\varepsilon^2 = \{\zeta \in \mathbb{C} : \arg\zeta = \pi - \varepsilon\}$ as well as $\gamma_\varepsilon^3 = \{\zeta \in \mathbb{C} : \arg\zeta = \varepsilon\}$. Together with the already computed integral over the arc $\gamma_{R,\varepsilon}^1$ we can conclude that in the limit $R \to \infty$

$$2\pi \mathrm{i}^{k+1} \sum_{j=1}^{N} m_j \alpha_j^k = -k(\pi - 2\varepsilon)\frac{\ell_k}{2^k \mathrm{i}^{k-1}} - k \int_{\gamma_\varepsilon^2 \oplus \gamma_\varepsilon^3} \zeta^{k-1} \left(\log d(\zeta) - \sum_{j=1}^{k-1} \frac{\ell_j}{(2\mathrm{i}\zeta)^j} \right) \mathrm{d}\zeta \,.$$

The left-hand side permits the limit $\varepsilon \to 0$ and thus we have proved the following trace formulae.

Theorem 4.3.3 *Let $V \in \mathcal{C}^\infty([0,b], \mathbb{R}^{m\times m})$ and consider the Schrödinger operator H with Dirichlet boundary conditions. Then the trace formulae*

$$\sum_{j=1}^{N} m_j |\mu_j|^{\frac{k}{2}} = \frac{k}{2\pi}(-i)^{k-1} \lim_{\varepsilon\to\infty} \int_{\gamma_\varepsilon^2 \oplus \gamma_\varepsilon^3} \zeta^{k-1} \left(\log d(\zeta) - \sum_{j=1}^{k-1} \frac{\ell_j}{(2\mathrm{i}\zeta)^j} \right) \mathrm{d}\zeta + \frac{(-1)^{k-1}k}{2^{k+1}} \ell_k$$

hold for every $k \in \mathbb{N}$.

For example, the first three trace formulae read

$$\begin{aligned}
&\sum_{j=1}^{N} m_j |\mu_j|^{\frac{1}{2}} = \frac{1}{2\pi} \lim_{\varepsilon\to 0} \int_{\gamma_\varepsilon^2 \oplus \gamma_\varepsilon^3} \log d(\zeta)\, \mathrm{d}\zeta - \frac{1}{4}\int_0^b \mathrm{tr}V(x)\, \mathrm{d}x, \\
&\sum_{j=1}^{N} m_j |\mu_j| \\
&= -\frac{\mathrm{i}}{\pi} \lim_{\varepsilon\to 0} \int_{\gamma_\varepsilon^2 \oplus \gamma_\varepsilon^3} \zeta \left(\log d(\zeta) + \frac{1}{2\mathrm{i}\zeta} \int_0^b \mathrm{tr}V(x)\, \mathrm{d}x \right) \mathrm{d}\zeta + \frac{1}{4}\big(\mathrm{tr}V(0) + \mathrm{tr}V(b)\big), \\
&\sum_{j=1}^{N} m_j |\mu_j|^{\frac{3}{2}} \\
&= -\frac{3}{2\pi} \lim_{\varepsilon\to 0} \int_{\gamma_\varepsilon^2 \oplus \gamma_\varepsilon^3} \zeta^2 \left(\log d(\zeta) + \frac{1}{2\mathrm{i}\zeta} \int_0^b \mathrm{tr}V(x)\, \mathrm{d}x + \frac{1}{(2\mathrm{i}\zeta)^2} \frac{1}{4}\big(\mathrm{tr}V(0) + \mathrm{tr}V(b)\big) \right) \mathrm{d}\zeta \\
&\quad + \frac{3}{16} \left(\mathrm{tr}V'(0) - \mathrm{tr}V'(b) + \int_0^b \mathrm{tr}V(x)^2\, \mathrm{d}x \right).
\end{aligned}$$

Note that the formulae have the desired symmetry properties. If we consider the new Schrödinger operator $\widehat{H}$ with potential $V(b-x)$, the eigenvalues remain unchanged and this is reflected in the trace identities.

Instead of $\gamma^2_{R,\varepsilon}$ and $\gamma^3_{R,\varepsilon}$ we could have used other paths which lie in the upper half-plane and which close the arc $\gamma^1_{R,\varepsilon}$ in such a way that all the $\mathrm{i}\alpha_j$ are contained in the interior. The only important property was that, as $|\zeta| \to \infty$ along the paths, $|\operatorname{Im}\zeta| \to \infty$ as well. We have chosen the rays with angles ε and $\pi - \varepsilon$ for simplicity.

We can use the exact same argument with a contour $\gamma'_{R,\varepsilon}$ that lies in the lower half-plane as described in Figure 4.2. With the definitions $\gamma^5_\varepsilon = \{\zeta \in \mathbb{C} : \arg\zeta = -\varepsilon\}$ as well as $\gamma^6_\varepsilon = \{\zeta \in \mathbb{C} : \arg\zeta = \varepsilon - \pi\}$ we then arrive at

$$2\pi(-\mathrm{i})^{k-1}\sum_{j=1}^{N} m_j\alpha_j^k = -k(\pi - 2\varepsilon)\frac{(-1)^k\ell_k}{2^k\mathrm{i}^{k-1}} - k\int_{\gamma^5_\varepsilon\oplus\gamma^6_\varepsilon}\zeta^{k-1}\left(\log d(\zeta) - \sum_{j=1}^{k-1}\frac{(-1)^j\ell_j}{(2\mathrm{i}\zeta)^j}\right)\mathrm{d}\zeta$$

and this implies that

$$\sum_{j=1}^{N} m_j|\mu_j|^{\frac{k}{2}} = -\frac{k}{2\pi}\mathrm{i}^{k-1}\lim_{\varepsilon\to 0}\int_{\gamma^5_\varepsilon\oplus\gamma^6_\varepsilon}\zeta^{k-1}\left(\log d(\zeta) - \sum_{j=1}^{k-1}\frac{(-1)^j\ell_j}{(2\mathrm{i}\zeta)^j}\right)\mathrm{d}\zeta + \frac{(-1)^{k-1}k}{2^{k+1}}\ell_k\,.$$

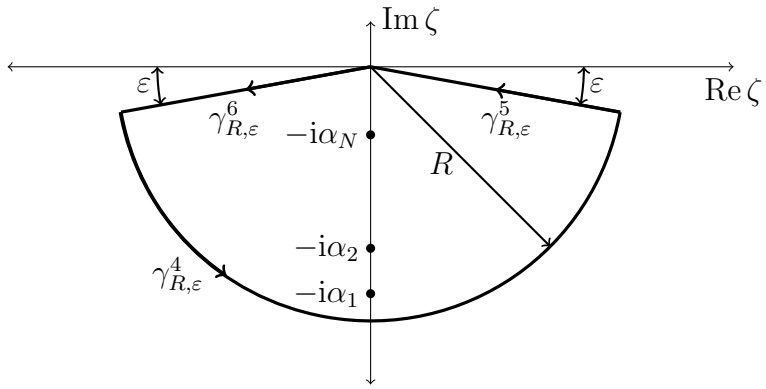


Figure 4.2: The contour $\gamma'_{R,\varepsilon} = \gamma^4_{R,\varepsilon} \oplus \gamma^5_{R,\varepsilon} \oplus \gamma^6_{R,\varepsilon}$

For example, the first three trace formulae read

$$\sum_{j=1}^{N} m_j|\mu_j|^{\frac{1}{2}} = -\frac{1}{2\pi}\lim_{\varepsilon\to 0}\int_{\gamma_\varepsilon^5\oplus\gamma_\varepsilon^6}\log d(\zeta)\,\mathrm{d}\zeta - \frac{1}{4}\int_0^b \mathrm{tr}V(x)\,\mathrm{d}x\,,$$

$$\sum_{j=1}^{N} m_j|\mu_j|$$

$$= -\frac{\mathrm{i}}{\pi}\lim_{\varepsilon\to 0}\int_{\gamma_\varepsilon^5\oplus\gamma_\varepsilon^6}\zeta\left(\log d(\zeta) - \frac{1}{2\mathrm{i}\zeta}\int_0^b \mathrm{tr}V(x)\,\mathrm{d}x\right)\mathrm{d}\zeta + \frac{1}{4}\big(\mathrm{tr}V(0)+\mathrm{tr}V(b)\big),$$

$$\sum_{j=1}^{N} m_j|\mu_j|^{\frac{3}{2}}$$

$$= \frac{3}{2\pi}\lim_{\varepsilon\to 0}\int_{\gamma_\varepsilon^5\oplus\gamma_\varepsilon^6}\zeta^2\left(\log d(\zeta) - \frac{1}{2\mathrm{i}\zeta}\int_0^b \mathrm{tr}V(x)\,\mathrm{d}x + \frac{1}{(2\mathrm{i}\zeta)^2}\frac{1}{4}\big(\mathrm{tr}V(0)+\mathrm{tr}V(b)\big)\right)\mathrm{d}\zeta$$
$$+\frac{3}{16}\left(\mathrm{tr}V'(0) - \mathrm{tr}V'(b) + \int_0^b \mathrm{tr}V(x)^2\,\mathrm{d}x\right).$$

Clearly these trace formulae are equivalent to the results of Theorem 4.3.3 by substituting ζ for $-\zeta$.

The obtained trace formulae can be compared to the identities (1.3) and (1.4). Note that, unlike the case of a Schrödinger operator on the real-line (or on the half-line), the function $\log d(\zeta)$ cannot be integrated over the real line $\mathrm{Im}\,\zeta = 0$. For this reason, it is not possible to decompose the integration of the function $\log d(\zeta)$ into an integration over the limit amplitude $a(\zeta) = |d(\zeta)|$ and a separate integration over the limit phase $\eta(\zeta) = \mathrm{Im}\,\log d(\zeta)$. The main difference is that in the case of a finite interval, the positive real axis is not covered with continuous spectrum, but contains an infinite number of eigenvalues. The roots of these eigenvalues are zeros of $d(\zeta)$ and thus the integration of $\log d(\zeta)$ along the real axis is impossible. As we will see in the next section, the integration has to be replaced with a summation over the singularities, which yields precisely the regularised trace formulae.

4.4 Recovering the Regularised Trace Formula

In this section we want to highlight how the obtained trace formulae are related to the result of Gel′fand and Levitan (1.2). In order to obtain the regularised trace formulae, we need to use the asymptotic behaviour of $\log d(\zeta)$ as derived in Theorem 4.2.2, without any assumptions on $\arg\zeta$. We use a similar argument as in [78].

For convenience, we denote by $\pm\beta_{j,0}$ the roots of the eigenvalues of H_0 counted with multiplicity m, such that

$$\beta_{mk,0} = \beta_{mk+1,0} = \cdots = \beta_{mk+m-1,0} = \frac{k\pi}{b}$$

for $k \geq 1$. Similarly, we denote the roots of the eigenvalues of H by $\pm\beta_j$, which are counted again with multiplicity. The first $2M = 2m_1 + \cdots + 2m_N$ numbers $\pm\beta_1, \ldots, \pm\beta_M$ lie on the imaginary axis and correspond to the negative eigenvalues $-\beta_j^2$. The remaining $\pm\beta_j$ lie on the real axis. Let $\delta > 0$ be smaller than π/b, which guarantees that no two distinct roots $(j\pi)/b$ of the free eigenvalues are within a distance of less than 2δ from each other. Consider now a sequence of circles with radii $R_n = \delta + n\pi/b$. Then there are $2mn$ roots $\pm\beta_{1,0}, \ldots, \pm\beta_{mn,0}$ in the interior of each circle (counted with multiplicity). Rouché's theorem together with the results of Theorem 4.2.1 implies that for sufficiently large n, there are also $2mn$ roots $\pm\beta_1, \ldots, \pm\beta_{mn}$ in the circle of radius R_n. Denoting by γ_n the counter-clockwise contour with $|\zeta| = R_n$, the residue theorem yields that

$$2\pi\mathrm{i}\big(1 + (-1)^k\big) \sum_{j=1}^{mn} (\beta_j^k - \beta_{j,0}^k) = -k \int_{\gamma_n} \zeta^{k-1} \log d(\zeta)\, \mathrm{d}\zeta\,.$$

Using the results of Theorem 4.2.2 we can conclude that

$$\begin{aligned} &2\pi\mathrm{i}\big(1 + (-1)^k\big) \sum_{j=1}^{mn} (\beta_j^k - \beta_{j,0}^k) \\ &= -k \int_{\gamma_n} \zeta^{k-1} \left(\sum_{j=1}^{k} \frac{1}{(2\zeta)^j} \left(\sum_{i=0}^{j} \ell_{i,j} \left(\frac{\cos \zeta b}{\sin \zeta b} \right)^i \right) + r(\zeta, k) \right) \mathrm{d}\zeta\,. \end{aligned} \tag{4.14}$$

Since we have proved in Theorem 4.2.2 that $|r(\zeta, k)| \leq C_k/|\zeta|^{k+1}$ for all $\zeta \in \Omega_\varepsilon$, the integral over the term $\zeta^{k-1} r(\zeta, k)$ vanishes as $n \to \infty$. It remains to compute integrals of the type

$$\int_{\gamma_n} \zeta^p (\cot \zeta b)^s \, \mathrm{d}\zeta$$

to derive the regularised trace formulae.

We first note that for odd $k \in 2\mathbb{N} - 1$ the left-hand side of (4.14) vanishes. As $d(\zeta) = d(-\zeta)$, the right-hand side is the integral of an even function over a circle and consequently

vanishes as well. The identity becomes trivial and we thus do not obtain regularised trace identities for half-integer powers of the eigenvalues. This is not surprising. It is (at least in the scalar case) well-known that the regularised trace has singularities at these half-integer points [23]. For even k, we obtain regularised trace identities for the Schrödinger operator with matrix-valued potential by computing the integrals.

Inside the circle γ_n, the function $\cot \zeta b$ has $(2n+1)$ singularities $\pm j\pi/b$ with $j = 0, 1, \dots, n$. The residues can be computed to be $1/b$. We thus obtain that

$$\int_{\gamma_n} \cot \zeta b \, \mathrm{d}\zeta = 2\pi \mathrm{i} \frac{1}{b}(2n+1)\,. \tag{4.15}$$

The residues of $\cot(\zeta)^2/\zeta$ at $\pm(j\pi)/b$ with $j \in \mathbb{N}$ can be commuted to be $-1/(j\pi)^2$ and the residue at 0 is found to be $-2/3$. As a consequence, we can conclude that as $n \to \infty$

$$\lim_{n\to\infty} \int_{\gamma_n} \frac{1}{\zeta} (\cot \zeta b)^2 \, \mathrm{d}\zeta = 2\pi \mathrm{i} \left(-\frac{2}{3} - \frac{2}{\pi^2} \sum_{j=1}^{\infty} \frac{1}{j^2} \right) = -2\pi \mathrm{i}\,, \tag{4.16}$$

where we have used the well-known fact that $\sum_{j=1}^{\infty} 1/j^2 = \pi^2/6$ (see e.g. [1, 23.2.24]). Combining (4.14) for $k = 2$ together with (4.15) and (4.16), as well as the fact that

$$\int_{\gamma_n} \frac{1}{\zeta} \, \mathrm{d}\zeta = 2\pi \mathrm{i}\,,$$

we can conclude that

$$2 \sum_{j=1}^{mn} (\beta_j^2 - \beta_{j,0}^2) = \frac{1}{b}(2n+1) \int_0^b \mathrm{tr} V(y) \, \mathrm{d}y - \frac{1}{2}\big(\mathrm{tr} V(0) + \mathrm{tr} V(b)\big) + r(n)$$

with some remainder $r(n)$ that converges to 0 as $n \to \infty$. By rearranging this equation such that only $r(n)$ and the terms independent of n remain on the right-hand side, we are able to take the limit $n \to \infty$ on this side. Consequently this limit must also exist on the left-hand side and thus we obtain that

$$\sum_{j=1}^{\infty} \left(\beta_j^2 - \beta_{j,0}^2 - \frac{1}{mb} \int_0^b \mathrm{tr} V(y) \, \mathrm{d}y \right) = -\frac{1}{4}\big(\mathrm{tr} V(0) + \mathrm{tr} V(b)\big) + \frac{1}{2b} \int_0^b \mathrm{tr} V(y) \, \mathrm{d}y\,.$$

We emphasise again that the convergence of the series on the left-hand side is a simple consequence of the convergence of the right-hand side. This identity is the generalisation

of (1.2) to the case of matrix-valued potentials. The same result was obtained in [13]. It is a special case of the formula derived in [39] for operator-valued potentials. In a similar way, regularised trace formulae for all integer powers of the eigenvalues μ_j can be obtained.

Chapter 5

The Berezin Inequality on Domains of Infinite Measure

This chapter is based on the published paper [64]. In [29] a similar result to the Berezin inequality (1.8) was established for the Dirichlet Laplace operator on a set Ω of infinite measure with complement $\mathbb{R}^d \setminus \Omega$ of finite measure. To this end one introduces the orthogonal projection $P_\Omega : L^2(\mathbb{R}^d) \to L^2(\Omega)$, i.e. the multiplication with the characteristic function χ_Ω. The operator $P_\Omega(-\Delta)P_\Omega$ corresponds to the Laplacian on the set Ω with Dirichlet boundary conditions. Since the continuous spectrum of $P_\Omega(-\Delta)P_\Omega$ contains the positive real axis, the operator $(P_\Omega(-\Delta)P_\Omega - \mu)_-$ is not trace-class on $L^2(\mathbb{R}^d)$. It can, however, be compared to a suitable operator to achieve similar results to (1.8) . The authors of [29] considered the difference $(-\Delta - \mu)_- - (P_\Omega(-\Delta)P_\Omega - \mu)_-$ and proved that (with the trace replaced by a regularised expression)

$$\operatorname{tr}\big((-\Delta - \mu)_- - (P_\Omega(-\Delta)P_\Omega - \mu)_-\big) \geq L^{\mathrm{cl}}_{1,d}|\mathbb{R}^d \setminus \Omega|\mu^{1+\frac{d}{2}}\,, \tag{5.1}$$

which can be seen as an analogue of the Berezin inequality for perturbations of the continuous spectrum of the Laplace operator. Bounds on traces for these types of problems are a fairly recent research area and we point to [29] for a generalisation of Lieb–Thirring inequalities to this setting.

In this thesis we aim to find an analogous inequality to (5.1) for the magnetic operator $H_B = (-\mathrm{i}\nabla + A(x))^2$. Similar to the case of the Laplacian, problems stem from the fact that $(P_\Omega H_B P_\Omega - \mu)_-$ is not trace-class. Thus we consider the difference $(H_B - \mu)_- - (P_\Omega H_B P_\Omega - \mu)_-$ and establish lower bounds on the trace of this operator. We also prove a

similar inequality for the sub-Laplacian L on the first Heisenberg group $\mathbb{H}^1$. A key observation for our results is that for any self-adjoint operator H, a formal computation involving the Berezin–Lieb inequality for convex functions (see [6] and [49]) yields the result

$$\operatorname{tr}\big((H-\mu)_- - (P_\Omega H P_\Omega - \mu)_-\big) \geq \operatorname{tr}\big((H-\mu)_- - P_\Omega (H-\mu)_- P_\Omega\big). \tag{5.2}$$

It is the object of this work to give correct mathematical meaning to this observation and to explicitly calculate the right-hand side for the two special choices of H.

We obtain lower bounds on the regularised traces of the differences $(H_B-\mu)_- - (P_\Omega H_B P_\Omega - \mu)_-$ and $(L-\mu)_- - (P_\Omega L P_\Omega - \mu)_-$ which are of the same form as the upper bounds in (1.10) and (1.11), respectively.

This chapter is organised as follows. In Section 5.1 we will discuss (5.2) in the general setting of H being a self-adjoint operator on $L^2(\mathbb{R}^d)$. We will state our main results for the magnetic operator H_B with constant magnetic field and the sub-Laplacian L in Theorem 5.1.3 and Theorem 5.1.4, respectively. The complete proofs of these results will be given in the subsequent sections.

5.1 Statement of the Main Results

We consider a separable Hilbert space $\mathcal{H}$ and let H be a self-adjoint operator on $\mathcal{H}$ with its spectral measure denoted by E. For $\mu \geq 0$ the spectral calculus allows us to define $(H-\mu)_-$ as

$$(H-\mu)_- = \int_{\mathbb{R}} (\mu - t)\chi_{(-\infty,\mu]}(t)\,\mathrm{d}E(t) = -(H-\mu)P_- \tag{5.3}$$

where we have used the notation $P_- = E((-\infty,\mu])$. Denote the complementary projection by $P_+ = \mathbb{I} - P_-$. We follow the definition of the relative kinetic energy in [29]. Let Q be a smooth, finite rank operator on $\mathcal{H}$. Clearly any operator A on $\mathcal{H}$ can be written as the sum of four operators corresponding to the decomposition of $\mathcal{H}$ into $\operatorname{ran}P_-$ and $\operatorname{ran}P_+$, i.e.

$$A = P_+AP_+ + P_+AP_- + P_-AP_+ + P_-AP_- \,.$$

In [58, Theorem VI.25] it is shown that, if T is trace-class and S is bounded, then $\mathrm{tr}(ST) = \mathrm{tr}(TS)$. Thus it holds that

$$\begin{aligned}\mathrm{tr}\big((H-\mu)Q\big) &= \mathrm{tr}\big(P_+(H-\mu)QP_+ + P_-(H-\mu)QP_-\big)\\ &= \mathrm{tr}\big(|H-\mu|P_+QP_+ - |H-\mu|P_-QP_-\big)\\ &= \mathrm{tr}\big(|H-\mu|^{\frac{1}{2}}(Q_{++}-Q_{--})|H-\mu|^{\frac{1}{2}}\big)\end{aligned}$$

where we have used the definitions $Q_{++} = P_+QP_+$ and $Q_{--} = P_-QP_-$. If we also assume that Q satisfies

$$-P_- \leq Q \leq P_+ \tag{5.4}$$

then clearly for all $x \in \mathcal{H}$

$$\langle QP_+x, P_+x\rangle = \langle (Q+P_-)P_+x, P_+x\rangle \geq 0\,.$$

As a consequence it holds that for all $x \in \mathcal{H}$

$$\langle Q_{++}x, x\rangle = \langle QP_+x, P_+x\rangle \geq 0$$

and thus $Q_{++} \geq 0$. Similarly it can be proved that (5.4) implies $Q_{--} \leq 0$ such that $Q_{++} - Q_{--} \geq 0$ and this shows that

$$\mathrm{tr}\big(|H-\mu|^{\frac{1}{2}}(Q_{++}-Q_{--})|H-\mu|^{\frac{1}{2}}\big) \geq 0$$

as long as (5.4) holds. This allows us to define a regularised trace which can only take values in $[0,+\infty]$.

Definition 5.1.1 *Let H be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$ and let Q be a bounded operator that satisfies (5.4). If $|H-\mu|^{\frac{1}{2}}Q_{\pm\pm}|H-\mu|^{\frac{1}{2}}$ are trace-class, then define*

$$\mathrm{tr}_0\big((H-\mu)Q\big) := \mathrm{tr}\big(||H-\mu|^{\frac{1}{2}}(Q_{++}-Q_{--})|H-\mu|^{\frac{1}{2}}\big)\,.$$

If one of the operators $|H-\mu|^{\frac{1}{2}}Q_{\pm\pm}|H-\mu|^{\frac{1}{2}}$ *is not trace-class then set*

$$\mathrm{tr}_0\big((H-\mu)Q\big) := +\infty\,.$$

This definition allows us to avoid any discussions about the existence of the traces under consideration. For an investigation of trace-class properties of similar types of differences of free and perturbed Schrödinger operators we refer to a recent paper [32]. If $(H-\mu)Q$ is trace-class then the definition of $\mathrm{tr}_0\big((H-\mu)Q\big)$ coincides with the definition of the usual trace on $\mathcal{H}$.

Let $\mathcal{H}$ now be $L^2(\mathbb{R}^d)$ and let Q be of the form $Q=\gamma-P_-$. As defined previously, $P_- = E((-\infty,\mu])$ with E denoting the spectral measure of a self-adjoint operator H on $\mathcal{H}=L^2(\mathbb{R}^d)$, and here γ is an operator such that $0\leq\gamma\leq P_\Omega$. The condition (5.4) is therefore satisfied. Following again [29] we observe that

$$Q_{--} = P_-(\gamma-\mathbb{I})P_- \leq P_-(P_\Omega-\mathbb{I})P_- = -P_-P_{\Omega^{\mathsf{c}}}P_-$$

and consequently the trace inequality

$$\mathrm{tr}_0\big((H-\mu)Q\big) = \mathrm{tr}\big(|H-\mu|^{\frac{1}{2}}(Q_{++}-Q_{--})|H-\mu|^{\frac{1}{2}}\big) \geq \mathrm{tr}\big((H-\mu)_-^{\frac{1}{2}}P_{\Omega^{\mathsf{c}}}(H-\mu)_-^{\frac{1}{2}}\big)\,.$$

holds, where $P_{\Omega^{\mathsf{c}}}=\mathbb{I}-P_\Omega$ is the multiplication with the characteristic function on the set Ω^{c} of finite measure. These results are summarised in the following theorem.

Theorem 5.1.2 *Let H be a self-adjoint operator on $L^2(\mathbb{R}^d)$. Then the Berezin–Lieb type inequality*

$$\mathrm{tr}_0\big((H-\mu)(\gamma-P_-)\big) \geq \mathrm{tr}\big((H-\mu)_-^{\frac{1}{2}}P_{\Omega^{\mathsf{c}}}(H-\mu)_-^{\frac{1}{2}}\big)$$

holds for all $0\leq\gamma\leq P_\Omega$ *and all* $\mu\geq 0$.

Let F be the spectral measure of $P_\Omega H P_\Omega$. Since P_Ω commutes with $P_\Omega H P_\Omega$, it holds that $F((-\infty,\mu])P_\Omega = P_\Omega F((-\infty,\mu])P_\Omega$ and consequently $0\leq F((-\infty,\mu])P_\Omega\leq P_\Omega$. By choosing γ to be $F((-\infty,\mu])P_\Omega$ and recalling (5.3), we can interpret the left-hand side of the inequality in Theorem 5.1.2 as a regularised expression for the trace of the difference $(H-\mu)_- - (P_\Omega H P_\Omega-\mu)_-$.

While this result is true for arbitrary self-adjoint operators H, we shall now apply it to two special choices of H to obtain the main results of this chapter. First, we consider

Schrödinger operators with magnetic fields. Let the magnetic field $B(x)$ be a two-form on $\mathbb{R}^d$ and the magnetic vector potential $A(x)$ a one-form satisfying $B(x) = \mathrm{d}A(x)$. We shall restrict ourselves to the case $d = 2$ and in the remainder of this chapter, we furthermore assume that B is constant and positive. Consider the magnetic operator $H_B = (-\mathrm{i}\nabla + A(x))^2$, which is defined as the closure of the form

$$\langle H_B\psi, \psi\rangle := \int_{\mathbb{R}^2} \big|\big(-\mathrm{i}\nabla + A(x)\big)\psi(x)\big|^2 \,\mathrm{d}x$$

on $\mathcal{C}_c^\infty(\mathbb{R}^2)$, the set of smooth functions with compact support. The obtained operator is found to be self-adjoint and the spectrum consists of eigenvalues $(2k+1)B$ for $k \in \mathbb{N}\cup\{0\}$. Each eigenvalue has infinite multiplicity and thus $(H_B-\mu)_-$ is not trace-class. The following result can be seen as a generalisation of the Berezin inequality.

Theorem 5.1.3 *Assume $d = 2$, $\mu \geq 0$, $B > 0$ and let Ω be an open subset of $\mathbb{R}^2$ such that $\mathbb{R}^2 \setminus \Omega$ has finite measure. Then for $0 \leq \gamma \leq P_\Omega$ the inequality*

$$\mathrm{tr}_0\big((H_B-\mu)(\gamma - P_-)\big) \geq \mathrm{tr}\big((H_B-\mu)_-^{\frac{1}{2}} P_{\Omega^{\mathrm{c}}} (H_B-\mu)_-^{\frac{1}{2}}\big) \tag{5.5}$$

holds and the right-hand side can be calculated explicitly as

$$\mathrm{tr}\big((H_B-\mu)_-^{\frac{1}{2}} P_{\Omega^{\mathrm{c}}} (H_B-\mu)_-^{\frac{1}{2}}\big) = |\mathbb{R}^2\setminus\Omega|\frac{B}{2\pi}\sum_{k=0}^{\infty}\big((2k+1)B-\mu\big)_- . \tag{5.6}$$

The proof of Theorem 5.1.3 is provided in Section 5.2. The lower bound (5.6) coincides with the upper bound (1.10) for the magnetic operator on the set Ω^{c} of finite volume. The proof will be the same.

Similar results can also be obtained on the first Heisenberg group $\mathbb{H}^1$. Here, $\mathbb{H}^1$ is considered to be the three-dimensional space $\mathbb{R}^3$ equipped with the non-commutative multiplication

$$(x_1,x_2,x_3)\circ(y_1,y_2,y_3) = \left(x_1+y_1, x_2+y_2, x_3+y_3 - \frac{1}{2}(x_1y_2 - x_2y_1)\right)$$

for $(x_1, x_2, x_3), (y_1, y_2, y_3) \in \mathbb{R}^3$. On the Heisenberg group, we introduce the two left-invariant vector fields

$$X_1 = \frac{\partial}{\partial x_1} + \frac{1}{2} x_2 \frac{\partial}{\partial x_3}, \quad X_2 = \frac{\partial}{\partial x_2} - \frac{1}{2} x_1 \frac{\partial}{\partial x_3}.$$

Using these definitions, we consider the quadratic form

$$\ell(\psi) = \int_{\mathbb{R}^3} \left(|X_1 \psi|^2 + |X_2 \psi|^2 \right) \mathrm{d}x_1 \, \mathrm{d}x_2 \, \mathrm{d}x_3$$

on $\mathcal{C}_c^\infty(\mathbb{R}^3)$ and note that the closure of this form gives the self-adjoint sub-Laplacian $L = -X_1^2 - X_2^2$ on $\mathbb{H}^1$. For a detailed background we refer to the literature, e.g. [11]. The spectrum of L is found to be continuous and it takes up the whole positive real axis. Thus $(L-\mu)_-$ is not trace-class but the sub-Laplacian L is found to satisfy the following analogue of the Berezin inequality.

Theorem 5.1.4 *Assume $\mu \geq 0$ and let Ω be an open subset of $\mathbb{R}^3$ such that $\mathbb{R}^3 \setminus \Omega$ has finite measure. Then for $0 \leq \gamma \leq P_\Omega$ the inequality*

$$\mathrm{tr}_0\big((L-\mu)(\gamma - P_-)\big) \geq \mathrm{tr}\big((L-\mu)_-^{\frac{1}{2}} P_{\Omega^\mathrm{c}} (L-\mu)_-^{\frac{1}{2}}\big) \tag{5.7}$$

holds for the sub-Laplacian L on $\mathbb{H}^1$ and the right-hand side can be calculated explicitly as

$$\mathrm{tr}\big((L-\mu)_-^{\frac{1}{2}} P_{\Omega^\mathrm{c}} (L-\mu)_-^{\frac{1}{2}}\big) = |\mathbb{R}^3 \setminus \Omega| \frac{1}{96} \mu^3 . \tag{5.8}$$

Similarly to the previous application, the lower bound (5.8) coincides with the upper bound (1.11) in the case of the Heisenberg sub-Laplacian being defined on the domain Ω^c of finite measure with Dirichlet boundary conditions. The proof of Theorem 5.1.4 is basically the same as in the case of finite measure [40] and can be found in Section 5.3. Note that this result can easily be generalised to the N-th Heisenberg group $\mathbb{H}^N$.

Theorem 5.1.2 can be used to prove the results of Frank, Lewin, Lieb and Seiringer [29] who show that

$$\mathrm{tr}_0\big((-\Delta-\mu)(\gamma - P_-)\big) \geq L^{\mathrm{cl}}_{\gamma,d} |\mathbb{R}^d \setminus \Omega| \mu^{1+\frac{d}{2}}$$

for the Laplacian $-\Delta$ on a set $\Omega \subset \mathbb{R}^d$ with complement of finite measure.

5.2 Proof of Theorem 5.1.3

Let $\varphi_\mu : \mathbb{R} \to \mathbb{R}$ be the convex function defined as

$$\varphi_\mu(t) = (t-\mu)_- = \begin{cases} \mu - t, & t \leq \mu \\ 0, & t > \mu\,. \end{cases} \tag{5.9}$$

Applying Theorem 5.1.2 to the operator H_B yields (5.5) and it only remains to prove (5.6). This has been done by Frank, Loss and Weidl [30]. For the convenience of the reader, we repeat the computations. The spectrum of H_B is entirely discrete and can be calculated to be $(2k+1)B$ for $k \in \mathbb{N} \cup \{0\}$. The projection onto the k-th Landau level is denoted by $\Pi_{B,k}$. The spectral theorem implies that the operator $\varphi_\mu(H_B)$ can then be written as

$$\varphi_\mu(H_B) = \sum_{k=0}^{\infty} \varphi_\mu\big((2k+1)B\big)\Pi_{B,k}\,.$$

We multiply this identity from both sides with the projection P_{Ω^c} and consider the trace of the obtained expression, i.e.

$$\operatorname{tr}\big(P_{\Omega^c}\varphi_\mu(H_B)P_{\Omega^c}\big) = \sum_{k=0}^{\infty} \varphi_\mu\big((2k+1)B\big)\operatorname{tr}(P_{\Omega^c}\Pi_{B,k})\,. \tag{5.10}$$

To explicitly calculate the summands on the right-hand side of (5.10), we observe that by the cyclicity of the trace

$$\operatorname{tr}(P_{\Omega^c}\Pi_{B,k}) = \operatorname{tr}(P_{\Omega^c}\Pi_{B,k}\Pi_{B,k}P_{\Omega^c}) = \|P_{\Omega^c}\Pi_{B,k}\|_{\sigma_2}^2\,, \tag{5.11}$$

where $\|\cdot\|_{\sigma_2}$ denotes the Hilbert–Schmidt norm. This norm can be calculated explicitly by using the integral kernel of the operator $P_{\Omega^c}\Pi_{B,k}$. Let $\Pi_{B,k}(x,y)$ be the integral kernel of $\Pi_{B,k}$ such that $\Pi_{B,k}\psi(x) = \int_{\mathbb{R}^2}\Pi_{B,k}(x,y)\psi(y)\,\mathrm{d}y$. There is an explicit formula for $\Pi_{B,k}(x,y)$ in terms of Laguerre polynomials (see e.g. [57]). We will use an approach, however, that only requires the explicit form of the diagonal $\Pi_{B,k}(x,x)$. The integral kernel of the composition $P_{\Omega^c}\Pi_{B,k}$ is given by

$$(P_{\Omega^c}\Pi_{B,k})(x,y) = \chi_{\Omega^c}(x)\Pi_{B,k}(x,y)\,.$$

We can calculate the Hilbert-Schmidt norm on the right-hand side of (5.11) by double integration of the square of the modulus of this integral kernel, i.e.

$$\operatorname{tr}(P_{\Omega^c}\Pi_{B,k}) = \|P_{\Omega^c}\Pi_{B,k}\|_{\sigma_2}^2 = \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} |\Pi_{B,k}(x,y)|^2 \chi_{\Omega^c}(x)\,\mathrm{d}y\,\mathrm{d}x\,. \tag{5.12}$$

To explicitly solve this integral, we point out some important properties of the function $\Pi_{B,k}(x,y)$. As the orthogonal projection $\Pi_{B,k}$ is self-adjoint it must hold that $\Pi_{B,k}(x,y) = \overline{\Pi_{B,k}(y,x)}$. By evaluating $\Pi_{B,k}$ at the delta distribution $\delta(x-x_0)$ and using the defining property of projections, $\Pi_{B,k} = \Pi_{B,k}\Pi_{B,k}$, it can easily be concluded that

$$\int_{\mathbb{R}^2} |\Pi_{B,k}(x_0,y)|^2\,\mathrm{d}y = \Pi_{B,k}(x_0,x_0)\,. \tag{5.13}$$

It is furthermore a remarkable fact that the diagonal of the integral kernel of $\Pi_{B,k}$ is given by the constant $\Pi_{B,k}(x,x) = \frac{B}{2\pi}$ for all $k \in \mathbb{N}\cup\{0\}$ (see e.g. [57] and the references therein). Using these properties, identity (5.12) can be continued as

$$\operatorname{tr}(P_{\Omega^c}\Pi_{B,k}) = \int_{\mathbb{R}^2} \Pi_{B,k}(x,x)\chi_{\Omega^c}(x)\,\mathrm{d}x = \frac{B}{2\pi}|\mathbb{R}^2\setminus\Omega|\,.$$

Inserting this equation back into (5.10) yields the final result

$$\operatorname{tr}\big(P_{\Omega^c}\varphi_\mu(H_B)P_{\Omega^c}\big) = |\mathbb{R}^2\setminus\Omega|\frac{B}{2\pi}\sum_{k=0}^{\infty}\varphi_\mu\big((2k+1)B\big)$$

which finishes the proof.

5.3 Proof of Theorem 5.1.4

Let the convex function $\varphi_\mu : \mathbb{R}\to\mathbb{R}$ be defined as in (5.9). Theorem 5.1.2 applied to L yields (5.7) and it only remains to show (5.8) which can be proved following calculations by Hansson and Laptev [40]. We will give their proof below. Firstly, we introduce the Fourier transformation $\mathcal{F}_{x_3}$ with respect to the variable x_3,

$$(\mathcal{F}_{x_3}\psi)(x_1,x_2,x_3) = (2\pi)^{-\frac{1}{2}}\int_{-\infty}^{+\infty} \mathrm{e}^{-\mathrm{i}x_3y_3}\psi(x_1,x_2,y_3)\,\mathrm{d}y_3\,.$$

A simple calculation shows that the Heisenberg sub-Laplacian L satisfies the identity

$$\mathcal{F}_{x_3} L \mathcal{F}_{x_3}^* = \left(\mathrm{i}\frac{\partial}{\partial x_1} - \frac{1}{2} x_2 x_3 \right)^2 + \left(\mathrm{i}\frac{\partial}{\partial x_2} + \frac{1}{2} x_1 x_3 \right)^2 . \tag{5.14}$$

For fixed x_3, the right-hand side of identity (5.14) can be identified with a two-dimensional Schrödinger operator with vector field $A = -\frac{x_3}{2}(-x_2, x_1)$. The corresponding magnetic field $B = \mathrm{d}A$ is constant and can be calculated to be $B = -x_3$. The eigenvalues of this magnetic operator H_{-x_3} are $(2k+1)|x_3|$ for $k \in \mathbb{N} \cup \{0\}$. Note that they depend on the variable x_3. Similar to the previous section we shall use the Landau projections $\Pi_{-x_3,k}$ to prove (5.8). With respect to the variable x_3, the operator $\mathcal{F}_{x_3} L \mathcal{F}_{x_3}^*$ simply acts as a multiplication operator and consequently the spectral theorem allows us to write

$$\varphi_\mu(\mathcal{F}_{x_3} L \mathcal{F}_{x_3}^*) = \sum_{k=0}^{\infty} \varphi_\mu\big((2k+1)|x_3|\big) \widehat{\Pi}_{-x_3,k} \tag{5.15}$$

where we have used the tensor product $\widehat{\Pi}_{-x_3,k} = \Pi_{-x_3,k} \otimes \mathbb{I}_{L^2(\mathbb{R})}$ with $\mathbb{I}_{L^2(\mathbb{R})}$ denoting the identity on $L^2(\mathbb{R})$. For convenience we introduce the notation $\mu_k(x_3) = \varphi_\mu\big((2k+1)|x_3|\big)$ omitting the dependence on μ for the moment. As a consequence of (5.15) we obtain the identity

$$\operatorname{tr}\big(P_{\Omega^c} \varphi_\mu(L) P_{\Omega^c}\big) = \sum_{k=0}^{\infty} \operatorname{tr}\big(P_{\Omega^c} \mathcal{F}_{x_3}^* \mu_k(x_3) \widehat{\Pi}_{-x_3,k} \mathcal{F}_{x_3} P_{\Omega^c}\big) . \tag{5.16}$$

This result can be compared to the analogous equation in the case of a magnetic operator (5.10). While in this setting the magnetic field was a given constant, we now consider a magnetic field that changes with the variable x_3. In addition, the Fourier transformation $\mathcal{F}_{x_3}$ has to be dealt with. The summands on the right-hand side of (5.16) can be written as Hilbert–Schmidt norms of certain operators, i.e.

$$\operatorname{tr}\big(P_{\Omega^c} \mathcal{F}_{x_3}^* \mu_k(x_3) \widehat{\Pi}_{-x_3,k} \mathcal{F}_{x_3} P_{\Omega^c}\big) = \Big\| P_{\Omega^c} \mathcal{F}_{x_3}^* \mu_k(x_3)^{\frac{1}{2}} \widehat{\Pi}_{-x_3,k} \Big\|_{\sigma_2}^2$$

for every $k \in \mathbb{N} \cup \{0\}$. Here we have used that the multiplication operator $\mu_k(x_3)$ and the projection $\Pi_{-x_3,k}$ commute. The investigation of these Hilbert–Schmidt norms requires us to calculate the integral kernels of the operators involved. Let $x = (x_1, x_2, x_3)$ and $y = (y_1, y_2, y_3)$ be two vectors in $\mathbb{R}^3$. The integral kernel of $P_{\Omega^c} \mathcal{F}_{x_3}^* \mu_k(x_3)^{\frac{1}{2}} \widehat{\Pi}_{-x_3,k}$ can

then be computed to be $\chi_{\Omega^c}(x)\frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}x_3y_3}\Pi_{-y_3,k}(x_1,x_2,y_1,y_2)\mu_k(y_3)^{\frac{1}{2}}$. As a consequence we obtain the identity

$$\begin{aligned}
&\left\|P_{\Omega^c}\mathcal{F}^*_{x_3}\mu_k(x_3)^{\frac{1}{2}}\widehat{\Pi}_{-x_3,k}\right\|^2_{\sigma_2}\\
&=\frac{1}{2\pi}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\chi_{\Omega^c}(x)|\Pi_{-y_3,k}(x_1,x_2,y_1,y_2)|^2\mu_k(y_3)\,\mathrm{d}y\,\mathrm{d}x\\
&=\frac{1}{2\pi}\int_{\mathbb{R}}\mu_k(y_3)\int_{\mathbb{R}^3}\chi_{\Omega^c}(x)\int_{\mathbb{R}^2}|\Pi_{-y_3,k}(x_1,x_2,y_1,y_2)|^2\,\mathrm{d}y_1\,\mathrm{d}y_2\,\mathrm{d}x\,\mathrm{d}y_3.
\end{aligned}$$

To calculate this integral, we recall (5.13) and stress again that the diagonal of the integral kernel $\Pi_{-y_3,k}(x_1,x_2,y_1,y_2)$ is known to be the constant $\frac{|y_3|}{2\pi}$. This results in

$$\begin{aligned}
\left\|P_{\Omega^c}\mathcal{F}^*_{x_3}\mu_k(x_3)^{\frac{1}{2}}\widehat{\Pi}_{-x_3,k}\right\|^2_{\sigma_2}&=\frac{1}{2\pi}\int_{\mathbb{R}}\mu_k(y_3)\int_{\mathbb{R}^3}\chi_{\Omega^c}(x)\frac{|y_3|}{2\pi}\,\mathrm{d}x\,\mathrm{d}y_3\\
&=\frac{1}{2\pi^2}|\mathbb{R}^3\setminus\Omega|\int_0^{+\infty}\big((2k+1)y_3-\mu\big)_-\,y_3\,\mathrm{d}y_3
\end{aligned}$$

where we have used the definition of $\mu_k(y_3)$ to obtain the last equality. We insert this identity back into (5.16) and substitute $p=(2k+1)y_3$ to conclude that

$$\begin{aligned}
\operatorname{tr}\big(P_{\Omega^c}\varphi_\mu(L)P_{\Omega^c}\big)&=\frac{1}{2\pi^2}|\mathbb{R}^3\setminus\Omega|\sum_{k=0}^{\infty}\frac{1}{(2k+1)^2}\int_0^{+\infty}\big(p-\mu\big)_-\,p\,\mathrm{d}p\\
&=\frac{1}{16}|\mathbb{R}^3\setminus\Omega|\int_0^{+\infty}\big(p-\mu\big)_-\,p\,\mathrm{d}p\,.
\end{aligned}$$

Here, the last equality follows from the well-known fact that $\sum_{k=0}^{\infty}\frac{1}{(2k+1)^2}=\frac{\pi^2}{8}$ (see e.g. [1, 23.2.28]). The remaining integral can be easily calculated to be

$$\int_0^{+\infty}\big(p-\mu\big)_-\,p\,\mathrm{d}p=\frac{\mu^3}{6}$$

and this yields the desired result.

Appendix A

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