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Spectral estimates for the magnetic Schrödinger operator and the Heisenberg Laplacian

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Abstract

In this thesis, which comprises four research papers, two operators in mathematical physics are considered.

The former two papers contain results for the Schrödinger operator with an Aharonov-Bohm magnetic field. In Paper I we explicitly compute the spectrum and eigenfunctions of this operator in $\mathbb{R}^2$ in a number of cases where a radial scalar potential and/or a constant magnetic field are superimposed. In some of the studied cases we calculate the sharp constants in the Lieb-Thirring inequality for $\gamma = 0$ and $\gamma \geq 1$.

In Paper II we prove semi-classical estimates on moments of the eigenvalues in bounded two-dimensional domains. We moreover present an example where the generalised diamagnetic inequality, conjectured by Erdős, Loss and Vougalter, fails. Numerical studies complement these results.

The latter two papers contain several spectral estimates for the Heisenberg Laplacian. In Paper III we obtain sharp inequalities for the spectrum of the Dirichlet problem in $(2n + 1)$-dimensional domains of finite measure.

Let λ_k and μ_k denote the eigenvalues of the Dirichlet and Neumann problems, respectively, in a domain of finite measure. N. D. Filonov has proved that the inequality $\mu_{k+1} < \lambda_k$ holds for the Euclidean Laplacian. In Paper IV we extend his result to the Heisenberg Laplacian in three-dimensional domains which fulfil certain geometric conditions.

Sammanfattning

I denna avhandling, som omfattar fyra forskningsartiklar, betraktas två operatorer inom den matematiska fysiken.

De båda tidigare artiklarna innehåller resultat för Schrödingeroperatorn med Aharonov-Bohm-magnetfält. I artikel 1 beräknas spektrum och egenfunktioner till denna operator i $\mathbb{R}^2$ explicit i ett antal fall då en radialsymmetrisk skalärvärd potential eller ett konstant magnetfält läggs till. I flera av de studerade fallen kan den skarpa konstanten i Lieb-Thirrings olikhet beräknas för $\gamma = 0$ och $\gamma \geq 1$.

I artikel 2 bevisas semiklassiska uppskattningar för moment av egenvärdena i begränsade tvådimensionella områden. Vidare presenteras ett exempel då den generaliserade diamagnetiska olikheten, framlagd som en förmodan av Erdős, Loss och Vougalter, är falsk. Numeriska studier kompletterar dessa resultat.

De båda senare artiklarna innehåller ett flertal spektrumuppskattningar för Heisenberg-Laplace-operatorn. I artikel 3 bevisas skarpa olikheter för spektret till Dirichletproblemet i $(2n + 1)$-dimensionella områden med ändligt mått.

Låt λ_k och μ_k beteckna egenvärdena till Dirichlet- respektive Neumannproblemet i ett område med ändligt mått. N. D. Filonov har bevisat olikheten $\mu_{k+1} < \lambda_k$ för den euklidiska Laplaceoperatorn. I artikel 4 visas detta resultat för Heisenberg-Laplaceoperatorn i tredimensionella områden som uppfyller vissa geometriska villkor.

Preface

Ei blot til lyst

Inscription in Det Kongelige Teater

This thesis, for the degree of Doctor of Philosophy in Mathematics, is an account of my research at the Department of Mathematics at the Royal Institute of Technology (KTH) in Stockholm between 2003 and 2007.

The thesis is divided into two parts. The first part is of an introductory character, and its main purpose is to provide a background and summary of the results presented in the appended four scientific papers, which constitute the second part and are referred to by roman numerals. Papers I and II are about magnetic Schrödinger operators. This subject area is introduced in Chapter 1, and the results contained in the papers are outlined in Chapters 2 and 3. Likewise, Chapter 4 introduces the mathematical setting of the Heisenberg Laplacian—this operator is studied in Papers III and IV—while Chapters 5 and 6 summarise the results presented therein.

Looking back at my four years at the department, I see a delightfully long line of people whom I would like to thank: my advisor Ari Laptev, for being an excellent guide to spectral theory and for sharing his deep knowledge and intuition for mathematics along with his light-heartedness and optimism; my co-author Rupert L. Frank, for being an inspiring mathematical example as well as a great friend; my fellow doctoral students, for our way of encouraging each other in uphill work by strong friendship and intellectual glamour. Outside KTH I owe many thanks to my loving family for their constant support.

Anders Hansson
Stockholm, November 2007

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(joint with R. L. Frank)
In: *Proceedings of Operator Theory, Analysis and Mathematical Physics 2006*, Birkhäuser, Basel, in press

Paper III

Sharp spectral inequalities for the Heisenberg Laplacian
(joint with A. Laptev)
In: *Groups and Analysis: The Legacy of Hermann Weyl*, Cambridge University Press, Cambridge, in press

Paper IV

An inequality between Dirichlet and Neumann eigenvalues of the Heisenberg Laplacian
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Chapter 1

Introduction to the magnetic Schrödinger operator

This chapter is intended as a background for Papers I and II. We first give a brief, and regrettably incomplete, review of the principles of quantum mechanics in its general form. We shall then explain the motivation for our study, the problem of proving the stability of matter, and how this is related to semiclassical estimates of the type which we prove. Finally, we discuss Schrödinger operators which model magnetic systems, particularly the Aharonov-Bohm field, and make a few remarks to facilitate reading.

In those sections which are of a historical character we do not include references to scientific publications. Among the numerous textbooks in this field we mention [13], as a conceptual and accessible overview, and [22], as a comprehensive reference on the mathematical techniques.

1.1 A non-relativistic quantum theory

The development of physics preceding quantum mechanics

Guided by the results of his famous experiments with scattering of alpha particles on gold foil, Ernest Rutherford proposed in 1911 his model of the atom as a positively charged, heavy nucleus surrounded by a cloud of negatively charged, light electrons. The model predicts that the observed scattering would be consistent with scattering of charged particles in a Coulomb potential. While the agreement with experiments was incontestable, the model suffered from the difficulty that no equilibrium position is possible for a system of charged particles. This serious flaw of the contemporary formulation of mechanics, by which the atom would collapse into a point in finite time, highlighted the need for a fundamentally new theory.

The increasing amount of spectral measurements of very high accuracy, notably by Gustav Robert Kirchhoff and Robert Bunsen, was an even more important incentive for the development of quantum mechanics. They discovered caesium and rubidium (atomic numbers 55 and 37) by spectral methods around 1860, and realised how their techniques could be applied to astrophysics. In 1885 Johann Jakob Balmer noted that the wavelengths of all known spectral lines of the hydrogen atom could be summarised by the formula

$$\frac{1}{\lambda} = R\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right), \qquad n_1, n_2 \in \mathbb{N}. \tag{1.1}$$

The constant R is named after Johannes Rydberg, who discovered the general version of this formula a few years later. Balmer's and Rydberg's considerations were still of a phenomenological nature, and the apparent structure expressed in their formulae could not be satisfactory explained before the establishment of what is today known as quantum mechanics.

The Schrödinger operator

The birth of quantum mechanics should be dated in 1925 or 1926. In 1925, Werner Heisenberg successfully applied matrix mechanics to calculate the energy eigenvalues of simple quantum systems, and Wolfgang Pauli used this theory to derive Balmer's so far empirical formula (1.1). The culmination of this development was Erwin Schrödinger's discovery, in 1926, of the equation named after him,

$$i\hbar\frac{\partial}{\partial t}\Psi = H\Psi, \tag{1.2}$$

where the *(reduced) Planck constant* $\hbar$ has dimensions energy $\times$ time and the *Schrödinger operator*

$$H = -\frac{\hbar^2}{2m}\Delta + V \tag{1.3}$$

plays the same role as the Hamiltonian function in classical analytical mechanics; V is the potential energy of the particle. The unknown Ψ, the *wave function*, is a complex-valued function of the configuration space coordinates. Following Max Born, one interprets $|\Psi(x,t)|^2$ (with the appropriate normalisation) as the probability density of finding the system at time t at point x in configuration space.

Experimental measurements of physical quantities correspond to the action of self-adjoint, time-invariant, linear operators, e.g., the position operator, $X\Psi(x,t) = x\Psi(x,t)$, and the momentum operator, $\hbar D\Psi(x,t) = -i\hbar\nabla_x\Psi(x,t)$. In addition to being the operator that governs time evolution of the system, the Schrödinger operator itself is associated with the total energy. Resuming the probabilistic interpretation, we understand

$$\langle A(t)\rangle = \int \Psi(x,t)^* A\Psi(x,t)dx \tag{1.4}$$

as being the expectation value of the physical quantity A at time t.

We make two remarks about the mathematical formalism. Firstly, instead of representing the physical observables by time-invariant operators (the *Schrödinger picture*), one may equally well include the time dependence into the operators while defining the wave function as a function of the coordinates only (the *Heisenberg picture*). Secondly, it is convenient to work in such units that $\hbar = 2m = 1$.

The Hamiltonian of a closed system (and of a system in a constant external field) cannot contain time explicitly, since all points in time are identical. Those points in configuration space at which the energy has definite values are called *stationary states* and are represented by eigenfunctions of the operator (1.3). Suppose the spectrum of H is discrete, i.e., $H\Psi_j = E_j\Psi_j$ for $j \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}$. We can then integrate the time-dependent Schrödinger equation (1.2) to obtain

$$\Psi_j(x,t) = e^{-iE_jt/\hbar}\psi_j(x), \tag{1.5}$$

where ψ_j is a function of the coordinates only. The expansion of an arbitrary wave function Ψ in terms of the wave functions of stationary states has the form

$$\Psi(x,t) = \sum_j c_j\Psi_j(x,t), \tag{1.6}$$

where $|c_j|^2$ is the probability of finding the system in the state Ψ_j. For normalisation we require $\sum_j |c_j|^2 = 1$. If the spectrum includes a continuous component (in this case the term ‘quantum mechanics’ is less evocative), a suitable form for (1.6) is

$$\Psi(x,t) = \int \Psi_s(x,t) dE_s, \tag{1.7}$$

where $\{\Psi_s : \ s \in \mathbb{R}\}$ is a family of states and E_s is a generalised function, the *spectral measure*, such that $\int dE_s = 1$.

Well-posedness

The works of Heisenberg and Schrödinger were not enough to make quantum mechanics a consistent mathematical theory; in fact, the crucial proof of existence of solutions did not appear until the 1940s. In response to the pioneering contributions, John von Neumann developed a theory of unbounded operators in Hilbert space precisely to deal with foundational questions in quantum mechanics. Von Neumann realised that the key to solving the time-depedent Schrödinger equation (1.2) is to prove that H is essentially self-adjoint, a problem which he, however, deemed to be impossibly hard for atomic potentials V (i.e., Coulomb potentials, see (1.9) below). The main compoments of the proof—a certain Sobolev inequality (this can be viewed as a quantitative version of the *uncertainty principle* in physics) and a perturbation-theory result by Franz Rellich—became available in the mid-1930s, but they were not put together until a decade later by Tosio Kato. (Interestingly enough, the corresponding classical problem is still open. Kato’s proof cannot be mimicked since the uncertainty principle does not have a counterpart outside quantum mechanics.)

A second consistency requirement is that quantum mechanics should contain classical mechanics as a special case. After all, quantum effects originate from the very small length scale of the studied objects, and it is not reasonable to expect a sharp borderline separating them from the world of macroscopic objects. This is indeed so. The transition to the limiting case of classical mechanics can be formally described as a passage to the limit $\hbar \to 0$ (cf. (1.5)), just like the transition from wave optics to geometrical optics corresponds to a passage to the limit of zero wavelength, $\lambda \to 0$. In general, the motion described by the wave function does not tend to motion in a definite path. Its connection with classical motion is that, if at some initial instant the wave function, and with it the probability distribution of the coordinates, is given, then at subsequent instants this distribution will change according to the laws of classical mechanics.

We end this general part of the introduction by noting that the Schrödinger operator is non-relativistic. It describes particles moving at small speeds compared to the speed of light c, and is, in a well-defined sense, the limit as $c \to \infty$ of the relativistic Dirac operator.

1.2 The stability of matter

Extensivity and stability

A fundamental property of fermionic matter is *extensivity*, that is, its size and energy content grows linearly with the number of particles. Combining two equal amounts of a gas or liquid gives a number of Coulomb interactions, be they repulsive or attractive, that is twice as large as the total number of interactions in the separate containers. The electrostatic energy cannot possibly be a linear function, but has to grow with the square of the number of particles. Since the universe does obviously not consist of a lump of particles sticking tightly together—this would be the case if the energy content of N particles were simply proportional to $-N^2$—there must be a mechanism that beats somehow the quadratic dependence of the binding Coulomb energy. This mechanism is Pauli's *exclusion principle*, a lower bound, linear in the number of particles, on the kinetic energy.

Lars Onsager was the first to raise this problem. Using as starting point the known fact from astrophysics that bulk matter in the absence of nuclear effects undergoes gravitational collapse, he asked how we know that bulk matter does not undergo 'electrostatic collapse'. Indeed, a system of one electron and one proton is easily seen to be stable in quantum mechanics (since the spectrum is bounded below), but it is not obvious *a priori* why an array of such systems does not collapse into a point. If the efforts of analysing this problem further by means of quantum mechanics had not led to a (partial) solution in agreement with our observations, this theory would probably have been regarded as much less relevant, or would even have been abandoned, by the scientific community.

We shall now make a mathematical definition of stability of matter. Let R_1, R_2, $\ldots$, R_K be the positions of the nuclei and $Z_1, Z_2, \ldots, Z_K$ their charges. These are considered fixed, for even in hydrogen, the nucleus is more than a thousand times heavier than the electron. We suppose that there are q species of fermions, i.e., the spin, or some equivalent non-spatial parameter, can assume q distinct values; in particular, $q = 2$ for electrons. Hence, every state can be occupied by at most q particles according to the exclusion principle. For the same reason, the wave function is antisymmetric in the sense that it changes sign on permutation of two particle labels. The total kinetic energy of a state Ψ, representing N particles, is given by

$$T_\Psi = \sum_{\sigma_1,\ldots,\sigma_N=1}^{q} \sum_{i=1}^{N} \int |\nabla_i \Psi(x_1,\ldots,x_N;\sigma_1,\ldots,\sigma_N)|^2 dx. \tag{1.8}$$

For particles located in $x = (x_1, x_2, \ldots, x_N) \in \mathbb{R}^{nN}$ the Coulomb interaction gives a total potential energy equal to

$$\begin{aligned} &V(x; R_1, \ldots, R_K) \\ &\quad = -\sum_{i=1}^{N}\sum_{k=1}^{K} \frac{Z_k}{|x_i - R_k|} + \sum_{1\le i<j\le N} \frac{1}{|x_i - x_j|} + \sum_{1\le k<l\le K} \frac{Z_k Z_l}{|R_k - R_l|} \end{aligned} \tag{1.9}$$

(units are chosen in order that $e = 1$). Note that the last term, by assumption, is a positive constant. The operator of multiplication by V gives the potential energy of the system, namely

$$U_\Psi = \sum_{\sigma_1,\ldots,\sigma_N=1}^{q} \int V(x)|\Psi(x;\sigma)|^2 dx. \tag{1.10}$$

In this notation, the energy of the *ground state* (the energy minimiser) is

$$\begin{aligned} &E_0(N, K, R_1, \ldots, R_K, q) \\ &\quad = \inf\left\{ T_\Psi + U_\Psi : \sum_{\sigma_1,\ldots,\sigma_N=1}^{q} \int |\Psi(x;\sigma)|^2 dx = 1,\ \Psi \text{ antisymmetric} \right\}. \end{aligned} \tag{1.11}$$

We distinguish between *stability of the first kind*,

$$\inf_{R_1,\ldots,R_K} E_0(N, K, R_1, \ldots, R_K, q) > -\infty, \tag{1.12}$$

and *stability of the second kind*,

$$\inf_{R_1,\ldots,R_K} E_0(N, K, R_1, \ldots, R_K, q) > -C(N + K), \tag{1.13}$$

where $C = C(Z_1, \ldots, Z_K, q)$.

Stability of the first kind was proved by Kato in the early 1960s, whereas the second problem is much harder and was solved by Freeman Dyson and Andrew Lenard in 1967. Their proof—in which the Pauli principle plays a decisive role, as one could expect—is relatively untransparent and yields a C so huge that (1.13) is meaningless from the point of view of an experimentalist. In 1975, Elliott Lieb and Walter Thirring presented an alternative proof of stability of the second kind, one that is more conceptual and the constant of which is roughly 10^{14} times smaller than that obtained by Dyson and Lenard. In the next section, we shall explain the salient points in their argument.

From eigenvalue inequalities to the stability of matter

Let $E_0, E_1, \ldots$ be the bound state energies (the negative eigenvalues) of the Schrödinger operator $-\Delta + V$ in $\mathbb{R}^n$, and suppose that their γth moment satisfies the *Lieb-Thirring inequality*,

$$\sum_j |E_j|^\gamma \leq R_{\gamma,n} \frac{1}{(2\pi)^n} \iint \left(|\xi|^2 + V(x)\right)_-^\gamma \, d\xi \, dx = R_{\gamma,n} L^{\mathrm{cl}}_{\gamma,n} \int V(x)_-^{\gamma+n/2} dx, \tag{1.14}$$

where $t_- = \max\{-t, 0\}$ and

$$L^{\mathrm{cl}}_{\gamma,n} = \frac{\Gamma(n+1)}{2^n \pi^{n/2} \Gamma(\gamma + \frac{n}{2} + 1)}. \tag{1.15}$$

The right-hand side of (1.14) measures the classical phase-space (position $\times$ momentum) of the system, where, heuristically speaking, every eigenstate occupies $(2\pi)^n$ units of volume. It turns out that the case relevant for proving stability of matter is $\gamma = 1$, but as we explain in Section 1 of Paper II, there is reason to study the validity of semi-classical estimates of this kind for any non-negative value of γ. Concerning the constant in (1.14) we note, firstly, that $R_{\gamma,n} \geq 1$ (this follows from Weyl-type asymptotics, see, e.g., [17, Ch. 12]) and, secondly, that $\gamma \mapsto R_{\gamma,n}$ is a non-increasing function [2]. It is known that $R_{\gamma,1}$ is finite for $\gamma \geq \frac{1}{2}$, $R_{\gamma,2}$ is finite for $\gamma > 0$ and $R_{\gamma,n}$ is finite for $\gamma \geq 0$ and all $n \geq 3$. In the case $\gamma = 0$, (1.14) is referred to as the *Cwikel-Lieb-Rozenblyum* inequality.

With inequality (1.14) at hand one proves the collective Sobolev inequality

$$\sum_{i=1}^{N} \int |\nabla_i \Psi(x_1, \dots, x_N)|^2 dx \geq \frac{K_{p,n}}{q^{2/n}} \left(\int \rho_\Psi(x_1)^{p/(p-1)} dx_1 \right)^{2(p-1)/n}, \tag{1.16}$$

where $\max\{\frac{n}{2}, 1\} \leq p \leq 1 + \frac{n}{2}$ for $n \neq 2$ (note that when $p = 1$, the right-hand side is to be interpreted as the supremum norm of ρ_Ψ) and $1 < p \leq 2$ for $n = 2$. $K_{p,n}$ is an explicit constant. We recognise the left-hand side as being the kinetic energy of a set of N fermions and

$$\rho_\Psi(x_1) = N \sum_{\sigma_1, \dots, \sigma_N = 1}^{q} \int |\Psi(x_1, x_2, \dots, x_N)|^2 dx_2 \cdots dx_N, \tag{1.17}$$

on the right-hand side, is the single-particle density. This is a major step in the proof of the operator inequality $H \geq -cN$, in other words (1.13); for a full account see [15].

We now demonstrate how extensivity follows in the particular case of N electrons ($q = 2$) moving in a quadratic potential. Filling the equidistant oscillator levels, the magnitude ω of the potential yet unspecified, we get

$$\frac{1}{2} \sum_{j=1}^{N} (-\Delta_j + \omega^2 \vec{x}_j^2) \geq \omega \frac{(3N)^{4/3}}{4} (1 + \mathcal{O}(N^{-1/3})). \tag{1.18}$$

We take the expectation value of the left-hand side using as Ψ the ground state of $-\Delta + V$, where V is given by (1.9) with $K = 1$. Moreover, we set

$$\omega = \frac{4}{(3N)^{4/3}} \left\langle -\sum_{j=1}^{N} \Delta_j \right\rangle \tag{1.19}$$

and we use the Virial theorem combined with (1.13),

$$2\langle T_\Psi \rangle + \langle U_\Psi \rangle = 0 \qquad \Rightarrow \qquad \left\langle -\sum_{j=1}^{N} \Delta_j \right\rangle = -E_0 \leq cN. \tag{1.20}$$

From (1.18) we then obtain

$$\left\langle \sum_{j=1}^{N} \vec{x}_j^2 \right\rangle \geq \frac{(3N)^{8/3}}{16 \left\langle -\sum_j \Delta_j \right\rangle} \geq cN^{5/3}, \tag{1.21}$$

so that $\langle \vec{x}_j^2 \rangle^{1/2} \geq cN^{1/3}$. As long as the Virial theorem is valid, i.e., as long as no external forces are applied, the system cannot shrink infinitely.

1.3 Magnetic Schrödinger operators

General properties

In order for (1.3) to describe the energy of a particle in an external magnetic field $\mathbf{B} : \mathbb{R}^n \to \mathbb{R}^n$, the Laplacian $\Delta = \nabla^2$ is replaced by $(\nabla - i\mathbf{A})^2$, where the *vector potential* $\mathbf{A} : \mathbb{R}^n \to \mathbb{R}^n$ satisfies $\operatorname{curl} \mathbf{A} = \mathbf{B}$. In general, $\mathbf{A}$ is not a bounded vector field and does not need to be smooth either. The latter fact is due to *gauge invariance*: we can add an arbitrary gradient $\nabla\chi$ to $\mathbf{A}$ and still get the same magnetic field $\mathbf{B}$. This reflects the intrinsic many-dimensionality of magnetism; any scalar $A(x)$ is itself the gradient of $\int_{x_0}^{x} A(s)ds$.

Since the gauge transformation $\psi \mapsto e^{-i\chi}\psi$ is unitary, and so does not alter the spectrum, gauge invariance rather eliminates than creates difficulties in spectral theory. One point of concern is how to make sense of $(\nabla - i\mathbf{A})$ and $(\nabla - i\mathbf{A})^2$ as operators in L^2. For $\psi \in L^2_{\mathrm{loc}}(\mathbb{R}^n)$ the appropriate condition to impose is $\mathbf{A} \in (L^2_{\mathrm{loc}}(\mathbb{R}^n))^n$, which ensures that every component of $(\nabla - i\mathbf{A})\psi$ is a distribution. It is customary to introduce, for a given $\mathbf{A}$, the *magnetic Sobolev space* $H^1_{\mathbf{A}}(\mathbb{R}^n)$, which consists of all functions $\psi : \mathbb{R}^n \to \mathbb{C}$ such that

$$\psi \in L^2(\mathbb{R}^n) \qquad \text{and} \qquad (\nabla - i\mathbf{A})\psi \in (L^2(\mathbb{R}^n))^n. \tag{1.22}$$

$H^1_{\mathbf{A}}$ is a Hilbert space for any $\mathbf{A} \in (L^2_{\mathrm{loc}}(\mathbb{R}^n))^n$ and C_0^∞ is a dense subset. In general, $H^1_{\mathbf{A}}(\mathbb{R}^n) \not\subseteq H^1(\mathbb{R}^n)$, but $\psi \in H^1_{\mathbf{A}}(\mathbb{R}^n)$ always implies $|\psi| \in H^1(\mathbb{R}^n)$; this follows by the celebrated *diamagnetic inequality*,

$$|\nabla|\psi|(x)| \leq |(\nabla - i\mathbf{A})\psi(x)| \qquad \text{for a.e. } x \in \mathbb{R}^n, \tag{1.23}$$

which holds provided $\psi \in H^1_{\mathbf{A}}(\mathbb{R}^n)$ with $\mathbf{A} \in (L^2_{\mathrm{loc}}(\mathbb{R}^n))^n$. For proofs see, e.g., [17].

The Aharonov-Bohm magnetic field

In Papers I and II we study the Aharonov-Bohm field, which can be described by an idealised macroscopic experimental situation. Consider an infinitely long solenoid, through which there is a constant magnetic flux $2\pi\alpha$ inside, and the radius of which tends to zero. This is a relevant model, e.g., for very thin impurities inside a superconductor. The limiting case is described, up to gauge transformations, by the vector potential $\mathbf{A}(x) = \alpha|x|^{-2}(-x_2, x_1)$. $\operatorname{curl}\mathbf{A}$ vanishes outside $(x_1, x_2) = (0, 0)$, but a quantum-mechanical particle will 'feel' a δ-type interaction. Movement parallel to the solenoid obeys classical mechanics, and we therefore disregard the x_3 coordinate. This phenomenon was first predicted in 1949 by Werner Ehrenberg and Raymond Siday [5] and, independently, in 1959 by Yakir Aharonov and David Bohm [1].

Any Aharonov-Bohm flux of unit magnitude can be removed by a gauge transformation using $\chi(x) = \arctan(x_1/x_2)$, but any non-integer multiple of this function is multivalued mod 2π. This quantisation effect is confirmed by the results in our papers, in the sense that letting α tend to the nearest integer will immediately bring us back to the non-magnetic situation.

Chapter 2

Overview of Paper I and additional results

The search for explicit solutions is the oldest and most primitive path towards new knowledge in mathematical physics. The method has a narrow field of application, for it is only in exceptional cases that we can solve the relevant differential equations by exact methods. These systems can be studied in far more detail, both from a qualitative and quantitative point of view, than what general, abstract methods permit. The observed particularities of an exactly solvable system may seem like isolated pieces of information, but are in fact clues to understanding more complicated and realistic quantum-mechanical systems, which are likely to share many essential features with the exactly solvable case. The hydrogen atom and the harmonic oscillator may be quoted as two simple yet very rich examples.

In Paper I, *On the spectrum and eigenfunctions of the magnetic Schrödinger operator with Aharonov-Bohm magnetic field*, we explicitly calculate the spectrum and eigenfunctions of the magnetic Schrödinger operator in $L^2(\mathbb{R}^2)$ with Aharonov-Bohm vector potential and either quadratic or Coulomb scalar potential. Thus having complete knowledge of the spectrum, we determine the sharp constants in the Cwikel-Lieb-Rozenblyum and Lieb-Thirring inequalities.

The part of Paper I which is about exact solutions will be presented here together with some complementary material on other exactly solvable Aharonov-Bohm systems. Unless otherwise stated, the additions are generalisations achieved after the publication of the paper and have so far only

p	$\mathbf{A}^{(p)}(x)$	$V^{(p)}(x)$	$\mu_m^{(p)}$	$z^{(p)}(r)$
1	$\alpha\|x\|^{-2}(-x_2,x_1)+\frac{1}{2}B(-x_2,x_1)$	$\beta\|x\|^2$	$\frac{1}{2}\|\alpha-m\|$	$\frac{\sqrt{B^2+4\beta}}{2}r^2$
2	$\alpha\|x\|^{-2}(-x_2,x_1)$	$-\beta\|x\|^{-1}$	$\|\alpha-m\|$	$2\|E_{k,m}^{(2)}\|^{1/2}r$
3	$\alpha\|x\|^{-2}(-x_2,x_1)$	$-\beta\|x\|^{-2}$	n/a	n/a
4	$\alpha\|x\|^{-2}(-x_2,x_1)+\frac{1}{2}B(-x_2,x_1)$	0	$\frac{1}{2}\|\alpha-m\|$	$\frac{1}{2}Br^2$
5	$\alpha\|x\|^{-2}(-x_2,x_1)+\frac{1}{2}B(-x_2,x_1)$	-$\beta\|x\|^{-2}$	$\frac{\sqrt{(\alpha-m)^2-\beta}}{2}$	$\frac{1}{2}Br^2$

Table 2.1: Admissible $\mathbf{A}^{(p)}, V^{(p)}$ and corresponding parameters $\mu_m^{(p)}, z^{(p)}$

been presented at a poster session[1]. The main novelty is the introduction of a constant magnetic background field, generated by the extra term $\frac{1}{2}B(-x_2,x_1)$ in the vector potential. This is the content of Section 2.1 and spectral inequalities for these systems will be discussed in Section 2.2.

2.1 Exact solutions

Main result

The differential expression

$$H^{(p)} = (i\nabla + \mathbf{A}^{(p)})^2 + V^{(p)}, \tag{2.1}$$

where $\mathbf{A}^{(p)}$ and $V^{(p)}$ are given in Table 2.1, is initially defined on smooth functions with compact support but can be identified with a unique self-adjoint operator in $L^2(\mathbb{R}^2\setminus\{0\})$, the Friedrichs extension; we will not distinguish between them in the notation. This extension is the closure of $C_0^\infty(\mathbb{R}^2\setminus\{0\})$ with respect to the quadratic form

$$h^{(p)}[u] = \int_{\mathbb{R}^2}(|(i\nabla+\mathbf{A}^{(p)})u|^2 + V^{(p)}|u|^2)dx. \tag{2.2}$$

We will assume for definiteness that $B, \beta \geq 0$ and, for the reason of gauge invariance, that $0 < \alpha < 1$.

[1] The poster session was part of the workshop *Spectral Theory and Partial Differential Equations* held in July 2006 at the Isaac Newton Institute for Mathematical Sciences, Cambridge.

Before looking at the specific features of the studied operator we mention two interesting special cases. On one hand, $H^{(p)}$ with $\alpha \in \mathbb{Z}$ and $V \equiv 0$ is the Landau operator, see, e.g., [13, Sect. 112]. On the other hand, if $B = 0$ and $V \equiv 0$ then $H^{(p)}$ is the free Aharonov-Bohm operator, which is considered in Paper II. The latter operator turns out to be diagonalisable, as explained in the next chapter.

To exploit the radial symmetry we decompose the function space into subspaces parametrised by the angular momentum:

$$L^2(\mathbb{R}^2) = \bigoplus_{m\in\mathbb{Z}} \mathfrak{H}_m, \qquad \text{where } \mathfrak{H}_m := \{|x|^{-1/2} g(|x|) e^{im\theta} : \ g \in L^2(0,\infty)\}. \tag{2.3}$$

The action of $H^{(p)}$ in the subspace $\mathfrak{H}_m$ is

$$H_m^{(p)} := -\frac{d^2}{dr^2} + \frac{(\alpha-m)^2 - \frac{1}{4}}{r^2} + B(\alpha - m) + \frac{B^2 r^2}{4} + V^{(p)}(r), \tag{2.4}$$

where $B = 0$ if $p = 2$ or 3 and $r = |x|$. Accordingly, the quadratic form can be expressed $h^{(p)}[u] = \sum_{m\in\mathbb{Z}} h_m^{(p)}[u_m]$, where $u_m \in \mathfrak{H}_m$ and

$$h_m^{(p)}[u] = \int_0^\infty \left(|u'|^2 + \left[\frac{(\alpha-m)^2 - \frac{1}{4}}{r^2} + B(\alpha - m) \right.\right. \\ \left.\left. + \frac{B^2 r^2}{4} + V^{(p)}(r) \right] |u|^2 \right) dr. \tag{2.5}$$

The method of Friedrichs requires that the quadratic form be lower semibounded (this lower bound is preserved by the extension). Indeed, for $p = 1, 2$ or 4 we can verify this simply by applying to each $h_m^{(p)}$ the classical Hardy inequality,

$$\int_0^\infty \frac{|u|^2}{4x^2} dx \le \int_0^\infty |u'|^2 dx, \qquad u \in H_0^1(0,\infty). \tag{2.6}$$

The same holds for $p = 3$ if we assume $\beta \le \alpha^2$. In the non-obvious case $p = 5$ we prove in Section A.1

Lemma 2.1. *If $\beta \le \alpha^2$, then $h^{(5)} \ge C^{(5)} \|u\|_2^2$ with $C^{(5)} > -\infty$.*

If $\beta > \alpha^2$, then $h^{(5)}$ is not bounded below.

This is enough to make precise the statements of

Theorem 2.2. *The point spectrum and continuous spectrum of $H^{(p)}$ are, respectively,*

$$\sigma_p(H^{(1)}) = \{E^{(1)}_{k,m} :\ (k,m) \in \mathbb{N}_0 \times \mathbb{Z}\} \qquad \sigma_c(H^{(1)}) = \emptyset \tag{2.7}$$

$$\sigma_p(H^{(2)}) = \{E^{(2)}_{k,m} :\ (k,m) \in \mathbb{N}_0 \times \mathbb{Z}\} \qquad \sigma_c(H^{(2)}) = [0,\infty) \tag{2.8}$$

$$\sigma_p(H^{(3)}) = \emptyset \qquad \sigma_c(H^{(3)}) = [0,\infty) \tag{2.9}$$

$$\sigma_p(H^{(4)}) = \{E^{(4)}_{k,m} :\ (k,m) \in \mathbb{N}_0 \times \mathbb{Z}\} \qquad \sigma_c(H^{(4)}) = \emptyset \tag{2.10}$$

$$\sigma_p(H^{(5)}) = \{E^{(5)}_{k,m} :\ (k,m) \in \mathbb{N}_0 \times \mathbb{Z}\} \qquad \sigma_c(H^{(5)}) = \emptyset, \tag{2.11}$$

where

$$E^{(1)}_{k,m} = B(\alpha - m) + \sqrt{B^2 + 4\beta}(|\alpha - m| + 2k + 1) \tag{2.12}$$

$$E^{(2)}_{k,m} = -\beta^2(2|\alpha - m| + 2k + 1)^{-2} \tag{2.13}$$

$$E^{(4)}_{k,m} = B(2(\alpha - m)_+ + 2k + 1) \tag{2.14}$$

$$E^{(5)}_{k,m} = B(\alpha - m + \sqrt{(\alpha - m)^2 - \beta} + 2k + 1). \tag{2.15}$$

The eigenfunction corresponding to $E^{(p)}_{k,m}$ is

$$\phi^{(p)}_{k,m}(r,\theta) = \left(z^{(p)}(r)\right)^{\mu^{(p)}_m} L_k^{2\mu_m+1}\left(z^{(p)}(r)\right) e^{im\theta}, \tag{2.16}$$

where $L^\gamma_k(x) = \frac{(\gamma+1)_k}{k!}\,{}_1F_1(-k,\gamma+1;x)$ is the generalised Laguerre polynomial and $\mu^{(p)}_m$, $z^{(p)}$ are given in Table 2.1.

Proof. $p = 1, 2, 5$: Following the procedure in Paper I closely, we reduce the algebraic eigenvalue problem to the confluent hypergeometric differential equation [29],

$$-u'' + \left(\frac{\mu^2 - \frac{1}{4}}{z^2} - \frac{\lambda}{z} + \frac{1}{4}\right) u = 0, \tag{2.17}$$

and then single out those solutions which belong to the operator domain by looking at their asymptotic behaviour.

$p = 3$: $H^{(3)}_m$ is the spherical Bessel operator.

$p = 4$: This situation was treated in [7] but is also a special case of $H^{(1)}$ and $H^{(5)}$, namely that of $\beta = 0$. □

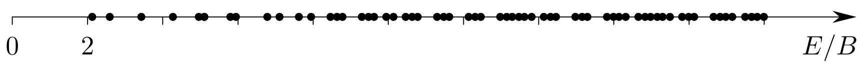

Figure 2.1: Point spectrum of $H^{(1)}$

A few further comments about the different spectra are in order. We will determine the multiplicities of the eigenvalues and discuss what impact the presence of the Aharonov-Bohm field has.

The spectrum of $H^{(1)}$

The eigenvalues of $H^{(1)}$ are related to the Landau levels in so far as the number
$$E^{(1)}_{k,m} - \sqrt{B^2 + 4\beta}(2k+1) \tag{2.18}$$
is independent of k. In other words, a new copy of the point spectrum is added at $\sqrt{B^2+4\beta}(2k+1)$ for every $k \in \mathbb{N}_0$. An example is shown in Figure 2.1. The only accumulation point is ∞. Two or more eigenvalues can coincide if $\sqrt{1+4\beta/B^2}$ is a rational number. Indeed, writing $\sqrt{1+4\beta/B^2} = p/q$, we have $E^{(2)}_{k,m} = E^{(2)}_{k',m'}$ if either

$$m > \alpha \quad \text{and} \quad \begin{cases} k' &= k - (p-q)l \\ m' &= m + 2pl \end{cases}, \qquad l = 0, 1, 2, \ldots, \left\lfloor \frac{k}{p-q} \right\rfloor, \tag{2.19}$$

or

$$m < \alpha \quad \text{and} \quad \begin{cases} k' &= k - (p+q)l \\ m' &= m - 2pl \end{cases}, \qquad l = 0, 1, 2, \ldots, \left\lfloor \frac{k}{p+q} \right\rfloor. \tag{2.20}$$

Hence, if this is the case, the multiplicities are

$$N(k,m) = \begin{cases} \left\lfloor \frac{k}{p-q} \right\rfloor + 1 & \text{if } m > \alpha, \\ \left\lfloor \frac{k}{p+q} \right\rfloor + 1 & \text{if } m < \alpha. \end{cases} \tag{2.21}$$

The special case $B = 0$ corresponds to the situation considered in Paper I, Theorem 2.1. It is convenient to write the eigenvalues as

$$E^{(1)}_{j,l}\big|_{B=0} = 2\sqrt{\beta}(\epsilon_j + l), \qquad j = 1, 2, \quad l \in \mathbb{N}_0, \tag{2.22}$$

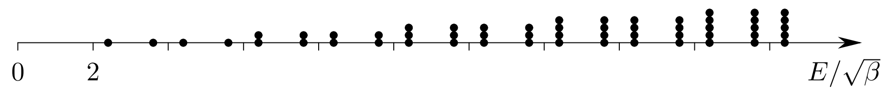

Figure 2.2: Point spectrum of $H^{(1)}$ if $B = 0$

where $\epsilon_1 = 1 + \{\alpha\}$, $\epsilon_2 = 2 - \{\alpha\}$, $\{\alpha\} = \alpha - \lfloor\alpha\rfloor$ and the multiplicities are given by

$$N^{(1)}(j,l) = \lfloor l/2 \rfloor + 1. \tag{2.23}$$

Clearly, there are only two simple eigenvalues. Looking at Figure 2.2, one may imagine that the spectrum has been derived from that of the harmonic oscillator by moving half of the eigenvalues in each point up and half of them (occasionally, but one) down a distance proportional to $\{\alpha\}$.

The spectra of $H^{(2)}$ and $H^{(3)}$

Both $H^{(2)}$ and $H^{(3)}$ have continuous spectrum on the positive real axis. The Coulomb potential $V^{(2)}(x) = -\beta|x|^{-1}$ gives rise to infinitely many bound states in the half-open interval $(-\beta^2, 0]$, whereas the inverse-square potential $V^{(3)}(x) = -\beta|x|^{-2}$ does not. Not surprisingly, the negative eigenvalues accumulate towards the continuous spectrum.

The spectrum of $H^{(4)}$

The spectrum of $H^{(4)}$ consists of the Landau levels $B(2k+1)$, $k \in \mathbb{N}_0$, interlaced by eigenvalues of finite multiplicity. The Landau levels are observed when a particle interacts with a constant magnetic field perpendicular to its plane of motion. A unified expression for the eigenvalues is $B(2(\alpha - m)_+ + 2k + 1)$ or, somewhat more transparently,

$$E^{(4)}_{j,l} = B(\epsilon_j + 2l), \qquad j = 1, 2, \quad l \in \mathbb{N}_0, \tag{2.24}$$

where $\epsilon_1 = 1$, $\epsilon_2 = 1 + 2(\alpha - m_0)$ and m_0 is that integer for which $0 < \alpha - m_0 < 1$. The multiplicities are given by

$$N^{(4)}(j,l) = \begin{cases} \infty & \text{if } j = 1, \\ l + 1 & \text{if } j = 2. \end{cases} \tag{2.25}$$

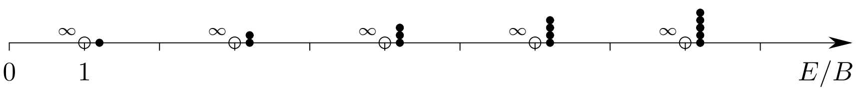

Figure 2.3: Point spectrum of $H^{(4)}$

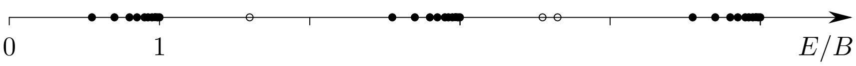

Figure 2.4: Point spectrum of $H^{(5)}$

As suggested by Figure 2.3, the $l+1$ eigenvalues in $E_{2,l}$ 'escaped from' the infinitely degenerate point $E_{1,l}$ as the Aharonov-Bohm field was added.

We have already announced that these observations were originally made in [7]. Some of the statements were extended in [21] to the case of arbitrarily many Aharonov-Bohm solenoids.

The spectrum of $H^{(5)}$

The way the Aharonov-Bohm field perturbs the Landau levels was described in the previous section. The addition of a scalar potential $-\beta|x|^{-2}$ gives us the operator $H^{(5)}$, the spectrum of which falls into two parts; see Figure 2.4 for an example.

Firstly, the indices $(1,k),(2,k),\ldots$ correspond to a monotone sequence of simple eigenvalues approaching $B(2k+1)$ from below. A Taylor expansion gives us

$$E^{(5)}_{k,m} = B(2k+1) + B|\alpha - m|\left(-1+\sqrt{1-\frac{\beta}{|\alpha-m|^2}}\right) \tag{2.26}$$

$$= B(2k+1) - \frac{\beta B}{2}\frac{1}{|\alpha-m|} + \mathcal{O}(|m|^{-3}) \qquad \text{as } m\to\infty. \tag{2.27}$$

The sequence begins in

$$B(\alpha - 1 + \sqrt{(\alpha-1)^2-\beta} + 2k+1) \geq B(\alpha+\sqrt{1-2\alpha}+2k) \geq B\left(2k+\frac{1}{2}\right) \tag{2.28}$$

and increases strictly with respect to m; one may realise this noting that

$$t \mapsto \alpha - t + \sqrt{(\alpha - t)^2 - \beta}, \tag{2.29}$$

is strictly increasing on $[\alpha + \sqrt{\beta}, \infty)$. This shows that the first component of the spectrum localises in $\bigcup_{k\in\mathbb{N}_0}[B(2k+1/2), B(2k+1))$ and that $B(2k+1)$ lies in the essential spectrum for all $k \in \mathbb{N}_0$.

Secondly, the introduction of the scalar potential turns the $(k+1)$-fold degenerate eigenvalue in $B(2\alpha + 2k + 1)$ into distinct points labelled by

$$\{(l, m) :\ l - m = k\} = \{(k, 0), (k-1, -1), \ldots, (0, -k)\}. \tag{2.30}$$

This is an increasing enumeration, so that all eigenvalues are simple. An increase of β does not split the eigenvalues apart, but rather pushes them down at different speeds:

$$dE_{k-l,-l} = -\frac{B}{2(\alpha + l)} d\beta. \tag{2.31}$$

By looking at the outermost eigenvalues we conclude that this second component of the spectrum is contained in

$$\begin{aligned} &\bigcup_{k\in\mathbb{N}_0} (B(\alpha + 2k + 1), B(2\alpha + 2k + 1)] \\ &\qquad \subset \bigcup_{k\in\mathbb{N}_0} (B(2k+1), B(2k+2)] \qquad \text{if } 0 < \alpha \leq \frac{1}{2}, \end{aligned} \tag{2.32}$$

$$\begin{aligned} &\bigcup_{k\in\mathbb{N}_0} \left[B(\alpha + \sqrt{2\alpha - 1} + 2k + 1), B(2\alpha + 2k + 1)\right) \\ &\qquad \subset \bigcup_{k\in\mathbb{N}_0} \left(B\left(2k + \frac{3}{2}\right), B(2k+3)\right] \qquad \text{if } \frac{1}{2} \leq \alpha < 1. \end{aligned} \tag{2.33}$$

We summarise the above discussion for clarity: For each $k \in \mathbb{N}_0$,

(i) the point $B(2k+1) \in \sigma_{\text{ess}}(H^{(5)})$;

(ii) the interval $[B(2k + \frac{1}{2}), B(2k+1))$ contains infinitely many simple eigenvalues;

(iii) the interval

$$\begin{cases} (B(2k+1), B(2k+2)] & \text{if } 0 < \alpha \leq \frac{1}{2}, \text{ or} \\ (B(2n + \frac{3}{2}), B(2n+3)] & \text{if } \frac{1}{2} \leq \alpha < 1 \end{cases} \tag{2.34}$$

contains $k+1$ simple eigenvalues;

(iv) the interval

$$\begin{cases} (B(2k+2), B(2k+\frac{5}{2})) & \text{if } 0 < \alpha \leq \frac{1}{2}, \text{ or} \\ (B(2k+1), B(2k+\frac{3}{2})) & \text{if } \frac{1}{2} \leq \alpha < 1 \end{cases} \tag{2.35}$$

is free of spectrum.

2.2 Spectral inequalities

With our complete knowledge of the spectrum it is a straightforward though lengthy procedure to determine the best constant R_γ in the two-dimensional Lieb-Thirring inequality,

$$\operatorname{tr}(H^{(p)} - \Lambda)_-^\gamma \leq \frac{R_\gamma}{(2\pi)^2} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} (|\xi|^2 + V(x) - \Lambda)_-^\gamma \, dx \, d\xi, \qquad \gamma \geq 0. \tag{2.36}$$

Assuming that $\sigma(H^{(p)}) \cap (-\infty, \lambda] = \{E_0, E_1, \ldots\}$ and carrying out the integration with respect to ξ, we obtain the equivalent inequality

$$\sum_j (E_j - \Lambda)_-^\gamma \leq R_\gamma L_{\gamma,2}^{\mathrm{cl}} \int_{\mathbb{R}^2} (V^{(p)}(x) - \Lambda)_-^{\gamma+1} dx. \tag{2.37}$$

Our subsequent discussion will concern $H^{(1)}$ with $B = 0$ and $H^{(2)}$.

The Cwikel-Lieb-Rozenblyum inequality ($\gamma = 0$)

If we specialise (2.37) to the operators under consideration, the right-hand side equals

$$R_\gamma \times \begin{cases} \dfrac{\Lambda^{\gamma+2}}{4\sqrt{\beta}(\gamma+1)(\gamma+2)} & \text{if } p = 1, \; B = 0, \quad \Lambda > 0, \\ \beta^2 \dfrac{\gamma\pi}{4\sin\gamma\pi} |\Lambda|^{\gamma-1} & \text{if } p = 2, \; \gamma < 1, \quad \Lambda < 0. \end{cases} \tag{2.38}$$

Maximising the quotient of the left- and right-hand sides with respect to Λ we get

Theorem 2.3. *For $p = 1$, $B = 0$, inequality* (2.36) *is sharp with*

$$R_0 = \begin{cases} \frac{2}{(1+|\alpha|)^2} & \text{if } 0 < |\alpha| \leq 3\sqrt{2} - 4, \\ \frac{1}{(1-\frac{1}{2}|\alpha|)^2} & \text{if } 3\sqrt{2} - 4 \leq |\alpha| \leq \frac{1}{2}. \end{cases} . \tag{2.39}$$

For $p = 2$, inequality (2.36) *is sharp with*

$$R_0 = \begin{cases} \frac{1}{(\frac{1}{2}+|\alpha|)^2} & \text{if } 0 < |\alpha| \le 2\sqrt{2} - \frac{5}{2}, \\ \frac{2}{(\frac{3}{2}-|\alpha|)^2} & \text{if } 2\sqrt{2} - \frac{5}{2} \le |\alpha| \le \frac{1}{2}. \end{cases} \tag{2.40}$$

We notice that $1 < R_\gamma(\alpha) \le \lim_{\alpha\to 0} R_\gamma(\alpha)$, which may be interpreted as a diamagnetic effect. The best known previous results were those of [19].

The Lieb-Thirring inequality ($\gamma > 0$)

It was shown in [3] (by a direct calculation) that $R_1 = 1$ for the *non-magnetic* harmonic oscillator $-\Delta + \beta|x|^2$. In Paper I we prove that the corresponding system with an Aharonov-Bohm field added does not need a larger constant. Hence, by known properties of the Lieb-Thirring constant, we have

Theorem 2.4. *For $p = 1$ and $B = 0$, inequality* (2.36) *is sharp with $R_\gamma = 1$ for all $\gamma \ge 1$.*

One may wonder whether the Lieb-Thirring constant is 'classical' already for a smaller exponent, i.e., whether there is a $\gamma_c < 1$ such that $R_{\gamma_c} = 1$. In [11] the authors prove that R_γ for $-\Delta + \beta|x|^2$ is non-classical for all $\gamma < 1$. Consequently, if we determined R_γ uniformly with respect to α, we would get the same answer, since this would also include the non-magnetic case. Numerical experiments give some support to the hypothesis that $\gamma_c < 1$ for non-integer α:

$\{\alpha\}$	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50
γ_c	0.85	0.82	0.77	0.73	0.63	0.70	0.74	0.76	0.76	0.77

Chapter 3

Overview of Paper II

In Paper II, *Eigenvalue estimates for the Aharonov-Bohm operator in a domain*, we study the Aharonov-Bohm operator

$$H_\alpha^\Omega = (i\nabla + \alpha\mathbf{A})^2 \qquad \text{in } L^2(\Omega), \tag{3.1}$$

where $\alpha \in \mathbb{R}$, $\mathbf{A}(x) = |x|^{-2}(-x_2, x_1)$ and $\Omega \subset \mathbb{R}^2$ is a domain of finite measure. (H_α^Ω can be seen as a magnetic Schrödinger operator, the potential of which forms a potential well, but since our analysis focuses on this special case, the chosen name is more appropriate.) Dirichlet boundary conditions are imposed on the boundary of Ω. More precisely, the operator (3.1) is defined through the closure of the quadratic form

$$\int_{\mathbb{R}^2} |(i\nabla + \alpha\mathbf{A})u|^2 dx, \qquad u \in C_0^\infty(\Omega \setminus \{(0,0)\}). \tag{3.2}$$

By gauge invariance, we only need to consider $0 < \alpha < 1$, but we have to assume that $(0,0)$ belongs to the simply-connected hull of Ω.

Just like in Paper I we decompose the space into

$$L^2(\mathbb{R}^2) = \bigoplus_{m\in\mathbb{Z}} \mathfrak{H}_m \qquad \text{with } \mathfrak{H}_m = \{|x|^{-1/2} g(|x|) e^{im\theta_x} : \ g \in L^2(0,\infty)\}. \tag{3.3}$$

The action of H_α on each subspace is

$$H_\alpha|_{\mathfrak{H}_m} \cong -\frac{d^2}{dr^2} + \frac{(m-\alpha)^2 - 1/4}{r^2}, \tag{3.4}$$

which we identify as the spherical Bessel operator. Therefore, we can diagonalise H_α by a unitary mapping $\mathcal{F}_\alpha$ with the following integral kernel:

$$\mathcal{F}_\alpha(\xi, x) = \frac{1}{2\pi} \sum_{m\in\mathbb{Z}} J_{|m-\alpha|}(|\xi||x|)e^{im(\theta_x-\theta_\xi)}, \tag{3.5}$$

where $x = |x|(\cos\theta_x, \sin\theta_x)$, $\xi = |\xi|(\cos\theta_\xi, \sin\theta_\xi)$ and J denotes the Bessel function of the first kind. The key property is

$$(\mathcal{F}_\alpha f(H_\alpha)u)(\xi) = f(|\xi|^2)(\mathcal{F}_\alpha u)(\xi), \qquad f \in L^\infty(\mathbb{R}). \tag{3.6}$$

The diagonalisation is in one sense the same kind of coincidence as the discovery of exact solutions; more precisely, the eigenfunctions of the studied operator defined in the whole plane are explicit. Note that $\mathcal{F}_0 = \mathcal{F}$ (cf. (4.2)) diagonalises the Laplacian $-\Delta$.

Hence, at least formally, $f(H_\alpha)$ is an integral operator with kernel

$$\begin{aligned} f(H_\alpha)(x, y) =& \int_{\mathbb{R}^2} \overline{\mathcal{F}_\alpha(\xi, x)} f(|\xi|^2)\mathcal{F}_\alpha(\xi, y)d\xi \\ =& \frac{1}{4\pi} \sum_{m\in\mathbb{Z}} \int_0^\infty J_{|m-\alpha|}(\sqrt{\lambda}|x|)f(\lambda)J_{|m-\alpha|}(\sqrt{\lambda}|y|)e^{im(\theta_x-\theta_y)}d\lambda. \end{aligned} \tag{3.7}$$

The trace of the operator is determined by the value on the diagonal of the kernel,

$$f(H_\alpha)(x, x) = \frac{1}{4\pi} \int_0^\infty f(\lambda)\rho_\alpha(\sqrt{\lambda}|x|)d\lambda, \tag{3.8}$$

where

$$\rho_\alpha(t) = \sum_{m\in\mathbb{Z}} J^2_{|m-\alpha|}(t), \qquad t \geq 0. \tag{3.9}$$

The quantity $\frac{1}{4\pi}\rho_\alpha(\sqrt{\lambda}|x|)$ is the local spectral density at energy λ.

3.1 Diamagnetic inequalities

Following Erdős, Loss and Vougalter [6] we ask which non-negative convex functions ϕ vanishing at infinity satisfy the 'generalised diamagnetic inequality',

$$\operatorname{tr} \chi_\Omega\phi(H_\alpha)\chi_\Omega \leq \operatorname{tr} \chi_\Omega\phi(-\Delta)\chi_\Omega \qquad \text{for all bounded domains } \Omega \subset \mathbb{R}^2. \tag{3.10}$$

Two important cases are $\phi(\lambda) = e^{-\lambda}$ and $\phi(\lambda) = (\lambda - \Lambda)_-^\gamma$, $\gamma \geq 1$, in the sense that the former follows immediately by (a stronger version, due to Kato) of the diamagnetic inequality (1.23) whereas there are two known counter-examples to the latter. By (3.8), inequality (3.10) is equivalent to the pointwise inequality

$$\int_0^\infty \phi(\lambda)\rho_\alpha(\sqrt{\lambda}r)d\lambda \leq \int_0^\infty \phi(\lambda)d\lambda \qquad \text{for all } r \geq 0. \tag{3.11}$$

By a detailed study of the function ρ_α we prove precise asymptotics of (3.8) as $|x| \to \infty$. This allows us to show that the generalised diamagnetic inequality is violated. We prove

Theorem 3.1. *Let $0 < \alpha < 1$ and let*

$$\phi(\lambda) = (\lambda - \Lambda)_-^\gamma \tag{3.12}$$

for some $\gamma \geq 1$, $\Lambda > 0$. Then the generalised diamagnetic inequality (3.10) *is violated. More precisely, there exist constants $C_1, C_2 > 0$ (depending on α and γ but not on Λ) such that, for all $|x| \geq C_1\Lambda^{-1/2}$,*

$$\left|\phi(H_\alpha)(x,x) - \phi(-\Delta)(x,x) + A_{\alpha,\gamma}(\Lambda)\frac{\sin(2\sqrt{\Lambda}|x| - \frac{1}{2}\gamma\pi)}{|x|^{\gamma+2}}\right| \leq C_2\frac{\Lambda^{(\gamma-1)/2}}{|x|^{\gamma+3}} \tag{3.13}$$

with $A_{\alpha,\gamma}(\Lambda) = (2\pi)^{-2}\Lambda^{\gamma/2}\Gamma(\gamma+1)\sin\alpha\pi$.

It is rather easy to construct a counterexample based on this result. Indeed, consider domains

$$\Omega_n = \{x \in \mathbb{R}^2 : \ |\sqrt{\Lambda}|x| - r_n| < \varepsilon\}, \qquad n \in \mathbb{N}, \tag{3.14}$$

with $r_n = \pi(n + \frac{1}{4}(\gamma - 1))$ and sufficiently small but fixed $\varepsilon > 0$.

The same analysis is used to prove the following positive result.

Proposition 3.2. *Let $0 < \alpha < 1$ and let ϕ be given by* (3.12) *for some $\gamma > -1$, $\Lambda > 0$. Then, for all open sets $\Omega \subset \mathbb{R}^2$,*

$$\operatorname{tr} \chi_\Omega\phi(H_\alpha)\chi_\Omega \leq R_\gamma(\alpha) \operatorname{tr} \chi_\Omega\phi(-\Delta)\chi_\Omega \tag{3.15}$$

with

$$R_\gamma(\alpha) = (\gamma+1)\sup_{r\geq 0}\int_0^1 (1-\lambda)^\gamma\rho_\alpha(\sqrt{\lambda}r)d\lambda. \tag{3.16}$$

The constant $R_\gamma(\alpha)$ above has to be evaluated numerically to the relevant accuracy. Here are a few approximate values:

	$R_\gamma(0.1)$	$R_\gamma(0.2)$	$R_\gamma(0.3)$	$R_\gamma(0.4)$	$R_\gamma(0.5)$
$\gamma = 0$	1.01682	1.03262	1.04422	1.05151	1.05397
$\gamma = \frac{1}{2}$	1.01027	1.02050	1.02781	1.03241	1.03395
$\gamma = 1$	1.00650	1.01351	1.01833	1.02138	1.02238
$\gamma = \frac{3}{2}$	1.00417	1.00920	1.01250	1.01457	1.01524
$\gamma = 2$	1.00267	1.00642	1.00874	1.01019	1.01065

Our approach also allows us to improve on the 'ordinary' diamagnetic inequality (1.23) for the Aharonov-Bohm operator. Since

$$r \mapsto \int_0^\infty e^{-\lambda} \rho_\alpha(\sqrt{\lambda} r) d\lambda \tag{3.17}$$

is a stricly increasing function on $[0, \infty)$, from 0 to 1, we have

Theorem 3.3. *$e^{-tH_\alpha}(x,x) < e^{-t(-\Delta)}(x,x)$ for all $x \in \mathbb{R}^2$.*

3.2 Semi-classical estimates

By the Berezin-Lieb inequality, Proposition 3.2 gives us the following semi-classical estimate, a magnetic counterpart of the Berezin-Li-Yau inequality.

Theorem 3.4. *Let $0 < \alpha < 1$, $\gamma \geq 1$ and $\Omega \subset \mathbb{R}^2$ be a bounded domain such that the operator H_α^Ω has discrete spectrum. Then, for any $\Lambda > 0$,*

$$\operatorname{tr}(H_\alpha^\Omega - \Lambda)_-^\gamma \leq \frac{R_\gamma(\alpha)}{(2\pi)^2} \int_{\Omega \times \mathbb{R}^2} (|\xi|^2 - \Lambda)_-^\gamma \, dx \, d\xi \tag{3.18}$$

with $R_\gamma(\alpha)$ as in (3.16)*.*

There is reason to believe that the use of the Berezin-Lieb inequality gives us a fairly crude estimate, and that actually, under the hypotheses of the theorem,

$$\operatorname{tr}(H_\alpha^\Omega - \Lambda)_-^\gamma \leq \frac{1}{(2\pi)^2} \int_{\Omega \times \mathbb{R}^2} (|\xi|^2 - \Lambda)_-^\gamma \, dx \, d\xi. \tag{3.19}$$

We challenge this hypothesis in a few numerical experiments, none of which falsifies it. More precisely, we study the quotient of the left- and right-hand sides of (3.18) as a function of Λ. While the primary aim of the experiments is to determine the value of $R_\gamma(\alpha)$, they also highlight how the quotient varies with respect to the magnitude α of the magnetic field and the volume and shape of Ω. The methods and results are described in the last section of the paper.

Chapter 4

Introduction to the Heisenberg Laplacian

In Papers III and IV, we prove eigenvalue estimates for the Heisenberg Laplacian, an operator which is also known as the Kohn Laplacian or sublaplacian. At least in the first paper, the estimates formally are Lieb-Thirring inequalities (1.14). We shall now place these results in a second, equally natural context by introducing the Heisenberg group and its associated Lie algebra of left-invariant vector fields.

For the most part, the papers are about operators associated with the first Heisenberg group $\mathbf{H}^1$ only. Please note that the simplified notation we use therein may not agree completely with that of this chapter.

4.1 Construction of the Heisenberg group

The nth Heisenberg group $\mathbf{H}^n$ is a natural object in two different mathematical contexts. On one hand, in complex function theory on the unit ball it can be identified with the group of translations of the Siegel upper half space,

$$S_{n+1} = \left\{ (z, z_{n+1}) \in \mathbb{C}^{n+1} : \; \operatorname{Im} z_{n+1} < |z|^2 \right\}. \tag{4.1}$$

This setting being somewhat outside the focus of the present thesis, we will not elaborate on it here but refer the interested reader to [28]. Instead, we will introduce $\mathbf{H}^n$ as the group generated by the exponentials of the two fundamental operators in quantum mechanics.

Exponentials of the position and momentum operators

The Fourier transform, as defined by

$$\mathcal{F}u(\xi) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-ix\cdot\xi} u(x)dx, \qquad \xi \in \mathbb{R}^n, \tag{4.2}$$

is a unitary operator in $L^2(\mathbb{R}^n)$. We shall now construct two more groups of unitary operators. The unbounded operators X_j, D_j, $j = 1, \ldots, n$, defined on a suitable space by

$$X_j u(x) = x_j u(x) \qquad \text{and} \qquad D_j u(x) = \frac{1}{i}\frac{\partial u}{\partial x_j}, \tag{4.3}$$

are called the *position* and *momentum* operators. For every $q, p \in \mathbb{R}^n$ we let

$$q \cdot X = \sum_{j=1}^{n} q_j X_j \qquad \text{and} \qquad p \cdot D = \sum_{j=1}^{n} p_j D_j, \tag{4.4}$$

for which the *Heisenberg commutator relation* holds,

$$[q \cdot X, p \cdot D] = i(q \cdot p)I. \tag{4.5}$$

The operator $q \cdot X + p \cdot D$ is essentially self-adjoint on both $C_0^\infty(\mathbb{R}^n)$ and the Schwartz space $\mathscr{S}(\mathbb{R}^n)$; for a proof see, e.g., [27]. Hence, by Stone's theorem [25], $\{m_q : \ q \in \mathbb{R}^n\}$ and $\{\tau_p : \ p \in \mathbb{R}^n\}$, where

$$m_q u(x) = e^{iq\cdot X} u(x) = e^{iq\cdot x} u(x) \qquad \text{and} \qquad \tau_p u(x) = e^{ip\cdot D} u(x) = u(x+p), \tag{4.6}$$

are groups of unitary operators. The Fourier transform intertwines these two groups: $\mathcal{F}\tau_p\mathcal{F}^{-1} = m_q$.

In order to derive the group structure we compare

$$\tau_p m_q u(x) = e^{iq\cdot(x+p)} u(x+p) \qquad \text{and} \qquad m_q \tau_p u(x) = e^{iq\cdot x} u(x+p), \tag{4.7}$$

from which the identity

$$e^{ip\cdot D} e^{iq\cdot X} = e^{ip\cdot q} e^{iq\cdot X} e^{ip\cdot D} \tag{4.8}$$

follows. This formula, which is indeed equivalent to (4.5), shows that all elements of the group generated by τ_p and m_q are of the form

$$e^{iq\cdot X} e^{ip\cdot D} e^{i(t+q\cdot p/2)} = e^{i(q\cdot X + p\cdot D + t)}, \qquad q, p \in \mathbb{R}^n, \ t \in \mathbb{R}. \tag{4.9}$$

In fact, the following important relation holds:

$$e^{i(q\cdot X+p\cdot D)}=e^{iq\cdot p/2}e^{iq\cdot X}e^{ip\cdot D}. \tag{4.10}$$

To see this, we let $H=q\cdot X+p\cdot D+t$ and compute the action of $\{e^{isH}\}_{s\in\mathbb{R}}$. If $v(s,x)=e^{isH}u(x)$, then

$$\left(\frac{\partial}{\partial s}-\sum_{j=1}^{n}p_j\frac{\partial}{\partial x_j}\right)v=i(q\cdot x+t)v \tag{4.11}$$

and $v(0,x)=u(x)$. This is satisfied by

$$v(s,x)=e^{i\left((q\cdot x+t)s+q\cdot p\frac{s^2}{2}\right)}u(x+sp), \tag{4.12}$$

and setting $s=1$ we obtain (4.10).

Applying (4.10) and the commutator identity (4.5) we obtain

$$\begin{aligned}&e^{i(q_1\cdot X+p_1\cdot D+t_1)}e^{i(q_2\cdot X+p_2\cdot D+t_2)}\\&\qquad=e^{i\left((q_1+q_2)\cdot X+(p_1+p_2)\cdot D+t_1+t_2+\frac{1}{2}(q_2\cdot p_1-q_1\cdot p_2)\right)}.\end{aligned} \tag{4.13}$$

We use this relation to define the nth Heisenberg group $\mathbf{H}^n$. Indeed, for every two points $(q_j,p_j,t_j)\in\mathbb{R}^n\times\mathbb{R}^n\times\mathbb{R}$,

$$(q_1,p_1,t_1)(q_2,p_2,t_2)=\left(q_1+q_2,p_1+p_2,t_1+t_2+\frac{q_2\cdot p_1-q_1\cdot p_2}{2}\right) \tag{4.14}$$

is a group operation. One easily verifies that $\mathbf{H}^n$, with identity $0=(0,0,0)$ and inverse $(q,p,t)^{-1}=(-q,-p,-t)$, is a Lie group.

Left-invariant vector fields

In the Heisenberg group there are $2n+1$ one-parameter subgroups given by

$$G_{2j-1}=\{(se_j,0,0):\ s\in\mathbb{R}\} \tag{4.15}$$

$$G_{2j}=\{(0,se_j,0):\ s\in\mathbb{R}\} \tag{4.16}$$

$$G_{2n+1}=\{(0,0,s):\ s\in\mathbb{R}\}, \tag{4.17}$$

where e_j, $1 \le j \le n$, are the coordinate vectors in $\mathbb{R}^n$. To each of these we associate a left-invariant vector field, namely

$$X_{2j-1} = \frac{\partial}{\partial q_j} - \frac{p_j}{2}\frac{\partial}{\partial t} \tag{4.18}$$

$$X_{2j} = \frac{\partial}{\partial p_j} + \frac{q_j}{2}\frac{\partial}{\partial t} \tag{4.19}$$

$$X_{2n+1} = \frac{\partial}{\partial t}. \tag{4.20}$$

These vector fields generate the Lie algebra $\mathfrak{h}_n$. The only non-zero commutator is $[X_{2j-1}, X_{2j}] = -X_{2n+1}$.

There is an interesting connection between the matrix representations of the Heisenberg group and its associated Lie algebra of vector fields. Set

$$m(x, y, z) = \begin{bmatrix} 1 & y^{\mathsf{T}} & t \\ 0 & I & x \\ 0 & 0 & 1 \end{bmatrix} \tag{4.21}$$

$$M(x, y, t) = m(x, y, t) - I, \qquad x, y \in \mathbb{R}^n,\ t \in \mathbb{R}. \tag{4.22}$$

We identify $\mathbf{H}^n$ with the group of matrices of the form $m(x, y, t + \frac{1}{2}x \cdot y)$, and $\mathfrak{h}_n$ is isomorphic to the Lie algebra of matrices $M(x, y, t)$ with the obvious Lie bracket. Now, a calculation shows that

$$e^{M(x,y,t)} = m\left(x, y, t + \frac{x \cdot y}{2}\right), \tag{4.23}$$

so the Heisenberg group is the image of its Lie algebra under the exponential map.

4.2 The Heisenberg Laplacian

An analogue of the Euclidean Laplacian

The Heisenberg Laplacian is the counterpart of the Laplacian on $\mathbb{R}^n$. In this capacity, it is a central object in the application of harmonic analysis on the Heisenberg group to partial differential equations. The Laplacian is characterised by

(i) invariance under translations and rotations,

(ii) homogeneity of degree 2,

and we shall now discuss what this signifies on the Heisenberg group. For every $g \in \mathbf{H}^n$ we have the left translation

$$L_g f(h) = f(g^{-1}h), \qquad h \in \mathbf{H}^n \tag{4.24}$$

and for every $\sigma \in U(n)$ the rotation

$$R_\sigma f(q,p,t) = f(\sigma(q,p),t), \qquad (q,p,t) \in \mathbf{H}^n. \tag{4.25}$$

(Explicitly, $\sigma(q,p) = (\sigma_1(q_1,p_1),\dots,\sigma_n(q_n,p_n))$, where $\sigma_j \in U(1)$.) An operator T acting on $\mathbf{H}^n$ is translation and rotation invariant if it commutes with L_g and R_σ for all $g \in \mathbf{H}^n$, $\sigma \in U(n)$. We recall that, in the Euclidean setting, T is homogeneous of degree α if

$$T(f(rx)) = r^\alpha (Tf)(rx), \qquad r > 0,\ x \in \mathbb{R}^n. \tag{4.26}$$

Instead of the isotropic dilation $x \mapsto rx$ we now consider $\delta_r(q,p,t) = (rq, rp, r^2 t)$, and (4.26) changes into

$$T(f(\delta_r g)) = r^\alpha T f(\delta_r g), \qquad r > 0,\ g \in \mathbf{H}^n. \tag{4.27}$$

It can be shown that up to a constant multiple, there is a unique differential operator on $\mathbf{H}^n$ satisfying (i) and (ii), namely the Heisenberg Laplacian (or sublaplacian, or Kohn Laplacian on $\mathbf{H}^n$).

Properties

The differential expression of the Heisenberg Laplacian is

$$A = -\sum_{j=1}^{2n} X_j^2, \tag{4.28}$$

where X_j are the left-invariant vector fields defined in the previous section. An explicit calculation shows that

$$A = -\Delta_{(q,p)} - \frac{|q|^2 + |p|^2}{2} \frac{\partial^2}{\partial t^2} + L \frac{\partial}{\partial t}, \tag{4.29}$$

where

$$L = \sum_{j=1}^{n} \left(q_j \frac{\partial}{\partial p_j} - p_j \frac{\partial}{\partial q_j} \right) \tag{4.30}$$

is the angular momentum operator in quantum mechanics.

Unlike the Laplacian $-\Delta$ in $\mathbb{R}^n$, A is not elliptic. This is not surprising if A is viewed as a Laplace-Beltrami operator, since the associated metric on $\mathbf{H}^n$ is a degenerated one. Nevertheless, A has the property of hypoellipticity (cf. [12, Th. 11.1.1]) and was shown to satisfy so-called subelliptic estimates by Gerald Folland and Joseph Kohn [9]. Among prominent contributions to the spectral theory of the Heisenberg Laplacian we mention those of Daryl Geller [10], Guy Métivier [20] and Robert Strichartz [26].

Chapter 5

Overview of Paper III and additional results

In Paper III, *Sharp spectral inequalities for the Heisenberg Laplacian*, we prove inequalities on the moments of the negative eigenvalues of the operators $A = -X_1^2 - X_2^2$ and $B = -X_1^2 - X_2^2 - X_3^2$, where X_1, X_2, X_3 are the left-invariant vector fields in $\mathbf{H}^1$. We recognise as A the Heisenberg Laplacian, whereas B is a related but elliptic operator which is not homogeneous of degree 2.

It is convenient to define a self-adjoint realisation of A using the quadratic form

$$a[u] = \int_{\mathbb{R}^3} \left(|X_1 u(x)|^2 + |X_2 u(x)|^2\right) dx, \tag{5.1}$$

which is initially defined for smooth functions with compact support. If $\Omega \subset \mathbb{R}^3$, then the closure of $C_0^\infty(\Omega)$ with respect to (5.1) corresponds to the Dirichlet realisation, $A_{\mathfrak{D}}$ or A_Ω, which is identified with A subject to Dirichlet boundary conditions on $\partial\Omega$. Likewise, the closure of $C^\infty(\bar{\Omega})$ is the Neumann realisation $A_{\mathfrak{N}}$. B is defined in a similar manner.

5.1 Spectral inequalities

Hypoelliptic case

Our main result is a Berezin-Li-Yau inequality.

Theorem 5.1. *Let $\Omega \subset \mathbb{R}^3$ be a domain of finite measure and let A_Ω be the operator A with Dirichlet boundary conditions in Ω. Then the spectrum of A_Ω consists of the eigenvalues $\lambda_0, \lambda_1, \ldots$, and*

$$\sum_{k=0}^{\infty} (\lambda - \lambda_k)_+ \leq \frac{1}{96} |\Omega| \lambda^3. \tag{5.2}$$

The proof is based on the fact that A is unitarily equivalent, under the partial Fourier transform, to a two-dimensional Laplacian with a constant magnetic field, *viz.*,

$$\begin{aligned} \mathcal{F}_3 A \mathcal{F}_3^* &= \left(i\partial_{x_1} - \frac{\xi_3}{2} x_2 \right)^2 + \left(i\partial_{x_2} + \frac{\xi_3}{2} x_1 \right)^2 & (5.3) \\ &= \left(i\nabla_{(x_1,x_2)} + \xi_3 \mathbf{A}(x_1,x_2) \right)^2, & (5.4) \end{aligned}$$

where $\mathbf{A}(x_1,x_2) = \frac{1}{2}(-x_2, x_1)$. Note that this is not a semi-classical phase-volume estimate; the right-hand side of such an inequality would have been infinite in this case.

From Theorem 5.1 we deduce

Corollary 5.2. *Under the conditions of Theorem 5.1 and for any $\gamma \geq 0$, the eigenvalues of A_Ω satisfy the Lieb-Thirring inequality*

$$\sum_{k=0}^{\infty} (\lambda - \lambda_k)_+^\gamma \leq K_\gamma \, |\Omega| \lambda^{\gamma+2} \tag{5.5}$$

with

$$K_\gamma = \begin{cases} \dfrac{9}{128} & \text{if } \gamma = 0, \\ \dfrac{9}{32} \dfrac{\gamma^\gamma}{(\gamma+2)^{\gamma+2}} & \text{if } 0 < \gamma \leq 1, \\ \dfrac{1}{16} \dfrac{1}{(\gamma+1)(\gamma+2)} & \text{if } 1 \leq \gamma. \end{cases} \tag{5.6}$$

We moreover prove that the inequality converse to (5.2) holds in the limit of large λ. Hence, the constant on the right-hand side is asymptotically sharp.

All the outlined estimates have analogues for the $\mathbf{H}^n$ Laplacian (4.28), and this is of course true for the subsequent results as well.

Elliptic case

The spectrum of B satisfies the semi-classical Lieb-Thirring inequality (1.14) with unit constant.

Theorem 5.3. *Let $\Omega \subset \mathbb{R}^3$ be a domain of finite measure and let B_Ω be the operator B with Dirichlet boundary conditions in Ω. Then the spectrum of B_Ω consists of the eigenvalues $\nu_0, \nu_1, \ldots$, and*

$$\sum_{k=0}^{\infty} (\lambda - \nu_k)_+ \leq \frac{1}{15\pi^2} |\Omega| \lambda^{5/2}. \tag{5.7}$$

5.2 A supplementary estimate

So far, we have restricted our study of the Dirichlet Heisenberg Laplacian A_Ω to the case where Ω is a domain of finite measure. Put differently, we have considered the Schrödinger-type operator $A - V$ for *potential wells*, i.e., with V being infinite outside and constant inside Ω. However, by heat-kernel methods we obtain the following upper bound on the counting function for potentials outside this class.

Theorem 5.4. *Let $N(A-V)$ be the number of negative eigenvalues of $A-V$. Then for any $V \in L^2(\mathbb{R}^3)$.*

$$N(A - V) \leq C \int_{\mathbb{R}^3} V(x)^2 dx \tag{5.8}$$

with

$$C = \min_{a>0} \frac{1}{32a} \frac{1}{e^{-a} + a\,\mathrm{Ei}(-a)} \geq 0.1886. \tag{5.9}$$

This result, the proof of which is deferred to Section A.2, is not an improvement in the case of potential wells; then already Corollary 5.2 gives us the constant $9/2^7 \approx 0.07031$.

Chapter 6

Overview of Paper IV

The main inequality in Paper IV, *An inequality between Dirichlet and Neumann eigenvalues of the Heisenberg Laplacian*, is not of a collective nature, and differs in this respect from those considered in the first three papers.

6.1 An eigenvalue inequality

The main result is true for two different geometrical hypotheses about the domain Ω. On one hand, we can assume that Ω can be written on the form

$$R_\sigma\Omega = \{(x_1, x_2, x_3) : \ a(x_2, x_3) < x_1 - \bar{x}_1 < b(x_2, x_3)\}, \\ \text{where } a(x_2, x_3) \le 0 \le b(x_2, x_3) \text{ for all } x_2, x_3 \quad (\dagger)$$

for some (x_1, x_2)-rotation $R_\sigma = \sigma \otimes I_3$, $\sigma \in U(1)$, and some $\bar{x}_1 \in \mathbb{R}$; and moreover,

$$\text{The cusps of } \Omega \text{ have at most power-like sharpness.} \quad (\ddagger)$$

On the other hand, we can also make the assumptions

$$\text{There exists } J \subset \mathbb{R}^2, \text{ card } J = \infty, \text{ such that for every } (\bar{x}_1, \bar{x}_2) \in J, \\ \text{all } x_3 \text{ sections of } \Omega \text{ are starshaped with respect to } (\bar{x}_1, \bar{x}_2). \quad (*)$$

and

$$\text{The embedding } H^1(\Omega) \subset L^2(\Omega) \text{ is compact.} \quad (**)$$

Condition $(\dagger)$ is slightly stronger than convexity in the x_1 direction, whereas $(*)$ may be seen as a kind of enhanced starshapedness.

Defining $A_{\mathfrak{D}}$ and $A_{\mathfrak{N}}$ as earlier, we can now state

Theorem 6.1. *Let $\Omega \subset \mathbb{R}^3$ be a domain of finite measure satisfying either (†), (‡) or $(*)$, $(**)$. Then $\mu_{k+1} < \lambda_k$ for all k, where λ_k and μ_k are the ordered eigenvalues of $A_{\mathfrak{D}}$ and $A_{\mathfrak{N}}$, respectively.*

The structure of the proof is close to that of Nikolay Filonov's paper [8], which studies the Euclidean Laplacian. The difficult part is finding a replacement, for each $\mu > 0$, for the set of complex exponential functions

$$\left\{ e^{i\langle\lambda,x\rangle} : \ \lambda \in \mathbb{C}, \ |\lambda|^2 = \mu \right\}. \tag{6.1}$$

Their key properties are

$$A\tau = \mu\tau, \tag{6.2}$$

$$\int_\Omega \left(|X_1\tau|^2 + |X_2\tau|^2\right) dx \leq \mu \int_\Omega |\tau|^2 dx. \tag{6.3}$$

It turns out that if (†), (‡) are imposed, we can use the family

$$\left\{ e^{-\frac{\mu}{2}[(x_1-\lambda)^2 + ix_2(x_1-2\lambda)]} e^{i\mu x_3} : \ \lambda \in I \right\} \tag{6.4}$$

where $I \subset \mathbb{R}$ is an interval of positive measure containing $\bar{x}_1$. In the case of $(*)$, $(**)$ we use instead

$$\left\{ e^{-\frac{\mu}{4}[(x_1-\lambda_1)^2 + (x_2-\lambda_2)^2 + 2i(x_1\lambda_2 - \lambda_1 x_2)]} e^{i\mu x_3} : \ \lambda \in J \right\} \tag{6.5}$$

with J as in $(*)$.

Appendix A

Proofs

A.1 Proof of Lemma 2.1

An application of Hardy's inequality (2.6) and the assumption $\beta \leq \alpha^2$ immediately gives us the estimate

$$h_m^{(5)}[f] \geq \int_0^\infty \left(B(\alpha - m) + \frac{B^2 r^2}{4} \right) |f|^2 dr \geq B(\alpha - m)\|f\|_2^2, \tag{A.1}$$

which is not uniform in m. However, it is possible to prove that $h_m^{(5)}[f] \geq -C\|f\|_2^2 \; \forall m \geq 5$, with $C > 0$ independent of m, which then yields $h^{(5)}[f] \geq C^{(5)}\|f\|_2^2$ with $C^{(5)} := \min\{-C, B(\alpha - 4)\}$. To this end we introduce $\chi_1, \chi_2 \in C_0^\infty(0, \infty)$ such that $0 \leq \chi_1, \chi_2 \leq 1$, $\chi_1^2 + \chi_2^2 \equiv 1$, $\operatorname{supp} \chi_1 \subset [0, R_2)$ and $\operatorname{supp} \chi_2 \subset (R_1, \infty)$, where

$$R_1 = \sqrt{\frac{2m\alpha}{B(\alpha + 1)}} \quad \text{and} \quad R_2 = \sqrt{\frac{2(m - 2\alpha)}{B}}. \tag{A.2}$$

Clearly, $R_1 < R_2 \; \forall m \geq 5$ and $R_2 - R_1 \to \infty$ as $m \to \infty$. By the IMS formula [4],

$$h_m^{(5)}[f] = h_m^{(5)}[\chi_1 f] + h_m^{(5)}[\chi_2 f] - \int_0^\infty (|\chi_1'|^2 + |\chi_2'|^2)|f|^2 dx, \tag{A.3}$$

with $\int (|\chi_1'|^2 + |\chi_2'|^2)|f|^2 dx \leq C||f||_2^2$ for some C independent of m. We now have

$$h_m^{(5)}[\chi_1 f] \geq \int_0^{R_2} \frac{(\alpha - m + \frac{1}{2}Br^2)^2 - \beta}{r^2} |\chi_1 f|^2 dr \tag{A.4}$$

$$\geq \int_0^{R_2} \frac{\alpha^2 - \beta + (2\alpha - m + \frac{1}{2}Br^2)(-m + \frac{1}{2}Br^2)}{r^2} |\chi_1 f|^2 dr \geq 0. \tag{A.5}$$

The other term can be estimated using that the lowest Landau level is B. Therefore, the corresponding quadratic form h_m^L satisfies

$$h_m^L[f] = \int_0^\infty \left(|f'|^2 + \frac{(-m + \frac{1}{2}Br^2)^2 - \frac{1}{4}}{r^2} |f|^2 \right) dr \geq B\|f\|_2^2. \tag{A.6}$$

Hence,

$$h_m^{(5)}[\chi_2 f] = h_m^L[\chi_2 f] + \int_{R_1}^\infty \frac{\alpha^2 - \beta + 2\alpha(-m + \frac{1}{2}Br^2)}{r^2} |\chi_2 f|^2 dr \tag{A.7}$$

$$\geq \int_{R_1}^\infty \left(B(\alpha + 1) - \frac{2m\alpha}{r^2} \right) |\chi_2 f|^2 dr \geq 0 \tag{A.8}$$

and we are done.

A.2 Proof of Theorem 5.4

Let (U, μ) be a σ-finite measure space. Any selfadjoint non-negative operator H in $L^2(U, \mu)$ generates a contractive semigroup $\{e^{-tH}\}_{t \in \mathbb{R}_+}$. We will assume that the corresponding integral kernel $e^{-tH}(x, y)$ is non-negative a.e. in $\mathbb{R}_+ \times U \times U$. Put

$$M_H(t) := \left\| e^{-tH/2} \right\|^2_{L^2 \to L^\infty} \tag{A.9}$$

and suppose this quantity is bounded for all $t > 0$, $M_H(t) = \mathcal{O}(t^\alpha)$, $\alpha > 0$ at zero and integrable at infinity. Moreover, let $G(s)$ be a function on $\mathbb{R}_+$, polynomially growing at infinity and such that $G(s)/s$ is integrable at $s = 0$. We associate to any such G the function

$$g(\sigma) := \int_0^\infty \frac{G(s)}{s} e^{-s/\sigma} ds. \tag{A.10}$$

(Note that $g(1/\sigma)$ is the Laplace transform of $G(s)/s$.) We shall apply the following bound on the counting function, which is sometimes called *Lieb's Formula*, see [16] or [23].

Theorem A.1. *Let H be an operator satisfying the hypotheses above and let $N(H-V)$ be the number of negative eigenvalues of $H-V$. For any $V \in L^2(U,\mu)$ and any admissible G,*

$$N(H-V) \leq \frac{1}{g(1)} \int_0^\infty \frac{1}{t} \int_U M_H(t) G(tV(x)) \mu(dx) dt. \tag{A.11}$$

When M_H is a homogeneous function, this statement can be simplified in the following way. Setting $M_H(t) = Kt^{-\nu/2}$ (and for ease of notation dx instead of $\mu(dx)$) and applying Fubini's theorem to the right-hand side, we find

$$\frac{K}{g(1)} \int_U \left(\int_0^\infty \frac{G(tV(x))}{t^{\nu/2+1}} dt \right) dx = \frac{K}{g(1)} \int_0^\infty \frac{G(s)}{s^{\nu/2+1}} ds \int_U V(x)^{\nu/2} dx. \tag{A.12}$$

In this case, (A.11) apparently is a (ν-dimensional) Cwikel-Lieb-Rozenblyum inequality, whose constant only depends on the exponent ν.

Proof of Theorem 5.4. It is easy to check that the operator A in $L^2(\mathbb{R}^3)$ fits into the framework described above, and so $N(A-V)$ can be estimated using Theorem A.1. Similarly to the proof of Theorem 5.1 we calculate, for $t > 0$, $x \in \mathbb{R}^3$,

$$\begin{aligned}
e^{-tA}(x,x) &= \left(\mathcal{F}_3^* e^{-t\mathcal{F}_3 A \mathcal{F}_3^*} \mathcal{F}_3 \right)(x,x) && \text{(A.13)}\\
&= \frac{1}{2\pi} \int_{-\infty}^\infty \sum_{n=0}^\infty e^{-\mu_n(\xi_3)t} \Pi_{\xi_3,n}(x,x) d\xi_3 && \text{(A.14)}\\
&= \frac{1}{2\pi^2} \sum_{n=0}^\infty \int_0^\infty e^{-\xi_3(2n+1)t} \xi_3 \, d\xi_3 && \text{(A.15)}\\
&= \frac{1}{2\pi^2 t^2} \sum_{n=0}^\infty \frac{1}{(2n+1)^2} \int_0^\infty e^{-s} s \, ds = \frac{1}{16t^2}. && \text{(A.16)}
\end{aligned}$$

This is exactly

$$M_A(t) = \operatorname*{ess\,sup}_{x \in \mathbb{R}^3} e^{-tA}(x,x), \tag{A.17}$$

so that $\nu = 4$. One can argue (see [16]) that the optimal G is of the form $G(s) = (s-a)_+$, $a > 0$. Now, since

$$\int_0^\infty \frac{G(s)}{s^{\nu/2+1}} ds = \frac{1}{2a} \tag{A.18}$$

and

$$g(1) = \int_a^\infty \left(1 - \frac{a}{s}\right) e^{-s} ds = e^{-a} + a \operatorname{Ei}(-a), \tag{A.19}$$

the best constant is the minimum of $[32a(e^{-a} + a \operatorname{Ei}(-a))]^{-1}$, as claimed. $\square$

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