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Quantum systems with magnetic field and point interactions

Ph.D. Thesis

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Contents

Chapter 1

Introduction

In this thesis, two physical systems are studied in the framework of non-relativistic quantum mechanics. While otherwise distinctly different, they have in common that both point interactions and magnetic fields are present in both of the systems.

The point interactions are described by singular potentials that are non-zero only on a discrete set (called singularity points in the 1- and 2-dimensional cases occuring in this thesis). Intuitively, the potentials can be described by δ-functions. In order to be applicable as Hamiltonians describing some systems, the operators with point interactions have to be given a rigorous sense as self-adjoint operators on Hilbert spaces, as described in detail in the book [AGHKH1]. The standard approach uses the theory of self-adjoint extensions of symmetric operators. The resulting operators can be described by some boundary conditions at singularity points. Different boundary conditions generally correspond to different physical situations.

We now turn our attention to the systems considered in this thesis. The first system describes the Aharonov-Bohm effect on the background of a homogeneous magnetic field. The frequently used idealized setup of the effect, allowing elegant treatment while leading necessarily to singular potentials, is considered.

The Aharonov-Bohm effect is a purely quantum phenomenon with huge influence on some fundamental aspects of quantum theory. Its essence lies in the observation that the motion of a charged particle is influenced by the existence of electromagnetic fields in the regions which the particle does not enter. Its significance lies in the conclusion that potentials, rather than fields, are the relevant entities in quantum mechanics, as contrasted with classical physics.

Introduced by Aharonov and Bohm in 1959 ([AB1]), the phenomenon attracted a lot of attention in the literature, with the original paper having

more than 2,700 citations. However, it was not until 1995 that the idealized setup was described rigorously by [DŠ] and [AT]. The key to the correct treatment of the system is the very definition of its Hamiltonians. Their singular potentials have to be precisely defined by the means of the aforementioned point interactions as done in the two papers. A four-parameter family of operators is necessary for the a description of the system.

A similar rigorous analysis of the Aharonov-Bohm effect in the presence of a homogeneous magnetic field was first provided in [EŠV]. The primary goals were to establish the boundary conditions defining the Hamiltonians, and to study their spectral properties.

The second system describes the H_2^+ molecule, an otherwise unstable object whose existence is made possible only by the presence of a strong homogeneous magnetic field. Such strong fields change the behavior of the matter dramatically, confining atoms and molecules into a very narrow cylindrical shape in the field direction, and rendering the models describing them effectively one-dimensional. Moreover, the existence of further otherwise unstable forms of matter is made possible. These fields appear e.g. on the surface of neutron stars.

The system is not explicitly solvable, leaving the investigation of even its basic properties to different variational, approximative or numerical techniques.

To surpass the insolvability, an approximative approach is developed in [BD3]. A "one-dimensional" operator with singular potential is constructed. The convergence to the Hamiltonian of the system in the resolvent norm sense is proved in the high field limit. The advantage is the precise knowledge of the bound on the error estimate.

In [BBjpa] and [BBfbs], the H_2^+ molecule is treated using this approach. The main goals are to established the convergence, and to study the ground state, the equilibrium distance of the nuclei and the energy of the system.

The core of the thesis is formed by the original results reported in three published articles [EŠV], [BBjpa] and [BBfbs]. The first paper regards the Aharonov-Bohm effect in the presence of a homogeneous magnetic field. The latter two papers concern H_2^+ molecule in a strong magnetic field.

As to the structure of the text, the point interactions are introduced in Chapter 2. Chapter 3 is devoted to the Aharonov-Bohm effect, and Chapter 4 concerns matter in strong magnetic fields.

Chapter 2

Point interactions

In this Chapter, we discuss a special class of quantum mechanical models; they are called point interaction models. These models are described by Hamiltonians with potential supported on a discrete set. One of their key features is that they are solvable – a quality allowing an explicit description of their spectrum, eigenfunctions and scattering properties.

These models are studied extensively in the literature, and they are used in an enormous number of applications. When properly defined, they can serve as approximations to more complicated unsolvable systems; their solvability renders them very useful in this role.

For a study of mathematically rigorous treatment of point interactions, the best reference is the book [AGHKH1]. Systems in one, two and three dimensions are described, with one, finite number as well as infinite amount of singularity points. For every situation, a rigorous way of treatment is described and some basic results are given. An extensive review of literature is provided as well.

In this thesis, two different types of point interaction models will occur. In Chapter 3, a two-dimensional system where the singularity is concentrated into one point is studied. In Chapter 4, a one-dimensional system with two points of singularity is used to describe H_2^+ molecule. We will discuss the methods for their correct definitions in Section 2.2 and Section 2.3, respectively, after giving some general description of point interactions in Section 2.1. Therein, we will adhere to the notation and terminology used in [AGHKH1].

2.1 General description of point interactions

As said, two examples of systems with point interactions will occur in this thesis. In their general form, these systems can be described in an intuitive way by formal operators of the type

$$H = -\Delta + \sum_{y \in Y} \lambda_y \delta_y(\cdot), \tag{2.1}$$

where Δ is the Laplacian with domain $H^{2,2}(\mathbb{R}^d)$ with $d = 1, 2, 3$; notice that Δ is self-adjoint as an operator on $L^2(\mathbb{R}^d)$. Further, $Y \subset \mathbb{R}^d$ is discrete (finite or countably infinite) set, with the points $y \in Y$ being called sources or points of singularity, λ_y is a coupling constant corresponding to y, and δ_y is a Dirac δ-function at y. In this way, one can regard the operators (2.1) as describing quantum particle moving under influence of singular, zero-range potential formed by sources of strength λ_y located at y.

Now, we will describe the idea that leads to the standard approach to the singular potentials in point interaction operators. We will consider the case where $Y = \{y\}$, thus $H = \Delta + \lambda\delta$. For every possible rigorous definition of H it must hold true that $H = -\Delta$ when restricted to the $C_0^\infty(\mathbb{R}^d \setminus \{y\})$. For $d \geq 4$ that would lead to the conclusion that $H = -\Delta$ on $H^{2,2}(\mathbb{R}^d)$ since $\Delta|_{C_0^\infty}(\mathbb{R}^d \setminus \{y\})$ is essentially self-adjoint. For $d = 2, 3$ it shows that there exist a one-parameter family of self-adjoint operators giving precise sense to $-\Delta + \lambda_y$, the parameter being some "renormalized coupling constans". This is mathematically formalized using Krein's theory of self-adjoint extensions.

As to the standard approach itself, the procedure is following. One starts with some symmetric operator; the singularity points are excluded from the supports of functions belonging to its domain. Then the theory of self-adjoint extensions is applied to the symmetric operator, yielding a family of operators. Each of these self-adjoint extensions is then described by some boundary condition applied to the functions from its domain at the points of singularity.

Let us note that the point interaction models do not restrict to the type defined above in (2.1) – some other systems can involve another type of point interaction such as δ'-interaction, or the multiparticle operators of the type

$$-\delta + \sum_{i<j}^{N} \lambda_{ij} \delta(x_i - x_j),$$

where λ_{ij} are coupling constants for the δ-interactions between i-th and j-th particles at x_i and x_j, respectively.

We will now turn our attention to the types of interaction used in the two systems we investigate in Chapter 3 and Chapter 4.

2.2 Point interactions in two dimensions

In this section, we will describe the correct treatment of the point interaction supported on one point of singularity in two dimensions. This model was studied in [AGHKH2], and the results appear in the book [AGHKH1] as well. The same approach is used in [DŠ] and [AT] to define the Hamiltonians that describe the Aharonov-Bohm effect in its idealized setup, see Section 3.3.3.

The goal here is to find a rigorous definition of the heuristic operator

$$H = -\Delta - \mu\delta(\cdot - y) \tag{2.2}$$

in $L^2(\mathbb{R}^2)$, where y denotes the point of singularity. According to the general discussion in the previous section, we should have $H\varphi = -\Delta\varphi$ for $\varphi \in C_0^\infty(\mathbb{R}^2)$ with $\varphi(y) = 0$, and therefore we can interpret (2.2) as a self-adjoint extension of

$$-\Delta|_{C_0^\infty(\mathbb{R}^2\setminus\{y\})}. \tag{2.3}$$

Let $\dot{H}_y$ be defined as the closure in $L^2(\mathbb{R}^2)$ of the operator (2.3). Then solving the equation

$$\dot{H}_y^*\psi(k) = k^\psi(k)$$

for

$$\dot{H}_y^* = -\Delta, \quad D(\dot{H}_y^*) = \left\{ g \in L^2(\mathbb{R}^2) \cap H^{2,2}_{loc}(\mathbb{R}^2 \setminus \{y\}) \;\middle|\; \Delta g \in L^2(\mathbb{R}^2) \right\}$$

shows that $\dot{H}_y$ has deficiency indices $(1,1)$. Then the decomposition of the Hilbert space is deployed,

$$L^2(\mathbb{R}^2, \mathrm{d}^2x) = \sum_{m\in\mathbb{Z}}^{\oplus} L^2(\mathbb{R}_+, r\,\mathrm{d}r) \otimes \mathbb{C}\, e^{\imath m\theta},$$

and the Hamiltonian $\dot{H}_y$ decomposes accordingly. Let l_m be formal operators

$$l_m = -\frac{d^2}{dr^2} + \frac{m^2 - \frac{1}{4}}{r^2}, \quad r > 0, m \in \mathbb{Z}.$$

Denoting $\dot{h}_m$ the restriction of $\dot{H}_y$ to sector m, we have that $\dot{h}_m = l_m$ for $r > 0, m \in \mathbb{Z}$, and

$$\begin{aligned} D(\dot{h}_m) &= \left\{ \varphi \in Ł^2(\mathbb{R}_+) \,\middle|\, \varphi, \varphi' \in AC_{\mathrm{loc}}(\mathbb{R}_+), l_m\varphi \in L^2(\mathbb{R}_+) \right\}, \quad m \neq 0, \\ D(\dot{h}_0) &= \left\{ \varphi \in Ł^2(\mathbb{R}_+) \,\middle|\, \varphi, \varphi' \in AC_{\mathrm{loc}}(\mathbb{R}_+), W(\varphi, \varphi_\pm), l_0\varphi \in L^2(\mathbb{R}_+) \right\}. \end{aligned}$$

Here W denotes the Wronskian, $W(g,h)_r = \overline{g(r)}h'(r) - \overline{g'(r)}h(r)$ and $\varphi_\pm$ are some functions.

Operator $\dot{h}_m$ is self-adjoint for $m \neq 0$, and $\dot{h}_0$ has deficiency indices $(1,1)$. Thus $\dot{h}_0$ has a one-parameter family of self adjoint extensions $h_{0,\alpha}$ for $\alpha \in (-\infty, \infty]$. It holds true that $h_{0,\alpha} = l_0$ and

$$D(h_{0,\alpha}) = \left\{ \varphi \in \text{Ł}^2(\mathbb{R}_+) \,\middle|\, \varphi, \varphi' \in AC_{\text{loc}}(\mathbb{R}_+), W(\varphi, \varphi_\pm), l_0\varphi \in L^2(\mathbb{R}_+), \right. \\ \left. 2\pi\alpha\varphi_0 + \varphi_1 = 0 \right\}, \quad \alpha \in (-\infty, \infty],$$

where

$$\varphi_0 = \lim_{r \downarrow 0} \left(r^{1/2} \ln r \right)^{-1} \varphi(r),$$
$$\varphi_1 = \lim_{r \downarrow 0} r^{-1/2} \left(\varphi(r) - 1\varphi_0(r) r^{1/2} \ln r \right),$$

for $\varphi \in D(h^*_{0,\alpha})$.

It can be seen that the self-adjoint extensions are determined by the boundary condition $2\pi\alpha\varphi_0 + \varphi_1 = 0$ that depends on the parameter α.

2.3 Point interactions in one dimension

In this section, we will depict the correct treatment of the point interaction model that will be used later to describe H_2^+ molecule. In fact, we will consider a more general setup with a finite number of point interactions in one dimension as done in [AGHKH1]. The definition of the H_2^+ will be provided in (4.19).

Let $N \in \mathbb{N}$ and let $Y = \{y_1, \ldots, y_N\} \subset \mathbb{R}$ be the set of sources. We define operator $\dot{H}_Y$ on $L^2(\mathbb{R})$ by

$$\dot{H}_Y = -\frac{d^2}{dx^2}, \qquad D(\dot{H}_Y) = \left\{ g \in H^{2,2}(\mathbb{R}) \,|\, g(y_j) = 0, y_j \in Y, j = 1, \ldots, N \right\}.$$

Operator $\dot{H}_Y$ is closed and has deficiency indices (N, N) which leads to a N^2-parameter family of self-adjoint extensions. In the same way as in [AGHKH1], we restrict ourselves to the case of so-called separated boundary conditions at each point y_j for $i = 1, \ldots, N$. This gives the following N-parameter family of self-adjoint extensions

$$\Delta_{\alpha,Y} = -\frac{d^2}{dx^2}, \tag{2.4}$$
$$D(\Delta_{\alpha,Y}) = \left\{ g \in H^{2,1}(\mathbb{R}) \cap H^{2,2}(\mathbb{R} \setminus Y) \,|\, g'(y_j+) - g'(y_j-) = \alpha_j g(y_j) \right\}.$$

Chapter 3

Aharonov-Bohm effect with a homogeneous magnetic field

This chapter is devoted to the study of the Aharonov-Bohm effect in the presence of a homogeneous magnetic field. Rigorous definition of Hamiltonians is given and the most general description of the system is derived, extending the results published in literature on this topic. An analysis of spectral properties is performed. One of its interesting and non-trivial implications is the fact that changes of parameters of point interactions lead to changes of spectra of the corresponding operators, showing the physical relevance of the approach. The results are summarized in paper [EŠV] that lies in the core of this part.

As to the structure of the text, in Section 3.1, the description of the Aharonov-Bohm effect as well as of its importance for quantum mechanics is given. The systems of interest are then rigorously defined in Section 3.2. Section 3.4 contains the actual results published in [EŠV]. Finally, Sections 3.3 and 3.5 are devoted to the review of literature showing the work in a broader research context. Here the former section concerns the preceding research while the latter covers the articles using or citing the results of [EŠV].

3.1 Aharonov-Bohm effect

The Aharonov-Bohm effect is a quantum-mechanical phenomenon wherein the motion of a charged particle is influenced by the existence of electromagnetic fields in the regions which the particle does not enter.

The history of the phenomenon dates from 1959 when Y. Aharonov and D. Bohm published their famous article "Significance of electromagnetic po-

tentials in the quantum theory" (cf. [AB1]); the phenomenon then came to be called the Aharonov-Bohm effect in their honor. However, it would be fair to remind that a magnetic type of the effect was first predicted already in 1949 by Ehrenberg and Siday, formulating electron optics by means of a refractive index represented by scalar and vector potentials (cf. [ES]).

We will discuss the phenomenon in detail in this section. Section 3.1.1 is devoted to the essence of the effect, while its history, experimental confirmation and implications to the quantum theory are described in Section 3.1.2.

Throughout this chapter, we will refer to the Aharonov-Bohm effect shortly as to the AB effect for the sake of convenience.

3.1.1 Significance of electromagnetic potentials in the quantum theory

The AB effect is of purely quantum character, not corresponding completely to any classical effect. In classical physics, the fundamental equations of motion can always be set up entirely by the means of fields, making the fields the only physically relevant entity. Vector and scalar electromagnetic potentials play the role of a convenient, yet dispensable mathematical tool for calculations related to fields.

However, in the quantum theory, the situation is different. One cannot get rid of the potentials in the Schrödinger eguation which suggests their possible physical significance. This is what Aharonov and Bohm realized and discussed in their article [AB1]. Therein, they proposed two electron interference experiments, too, that would show how the potentials influence electrons passing through field-free regions.

The main idea is the same for both experiments. An electron beam comes from the left and is split into two parts. Each of the two halves passes through some region where no field is present, both parts then are reunited at the right to form an interference pattern. Any change in the relative phase between the two beams will cause a shift in the interference pattern. In case of no external influence on the electrons, the pattern will be determined solely by the length difference of the two paths.

Then the electric or magnetic field is added as seen in Fig. 3.1 and Fig. 3.2 later on. In both cases, the setup ensures that any contact between the field and the beams is avoided. Despite that, the phase shift between the two beams occurs, which leads to observable changes of the interference pattern. Evidently, there is a change in the physical situation.

As can be seen, the nature of the AB effect is of a dual character and can

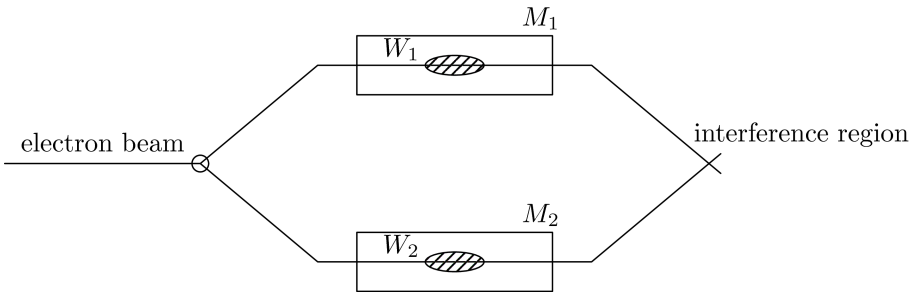

Figure 3.1: Electric AB effect. W_1, W_2 wave packets, M_1, M_2 metal cylinders.

be categorized into electric and magnetic effects. We will now discuss both of them.

Electric AB effect

We begin first with a simple example. We consider a charged particle inside a "Faraday cage" connected to a generator that makes the potential on the cage change in time; inside the region, the potential is a function of time only. Let us denote by H and H_0 respectively the Hamiltonian of the system with the generator on and off, i.e. $H = H_0 + e\varphi$, where $\varphi = \varphi(t)$ is the mentioned time-dependent scalar potential. Let ψ and ψ^0, respectively, be the solution of the corresponding Schrödinger equation. Then we have a relationship between ψ and ψ^0 reading

$$\psi = \psi^0 e^{-\imath S/\hbar}, \qquad S = e \int \varphi \, \mathrm{d}t,$$

which follows from

$$\imath\hbar \frac{\partial \psi}{\partial t} = \left(\imath\hbar \frac{\partial \psi^0}{\partial t} + \psi^0 \frac{\partial S}{\partial t} \right) e^{-\imath S/\hbar} = (H_0 + e\varphi)\, \psi = H\psi.$$

The only difference between the wave functions is the phase factor $e^{-\imath\hbar S}$ which has no physical consequences as to the observable results of measuring; both ψ and ψ^0 lie in the same one-dimensional subspace of Hilbert space, thus determining the same state of the system. However, this example shows us a route to the actual electric AB effect.

The setup of the thought experiment is schematically illustrated in Fig. 3.1. An electron wave packet is split into two (we will talk about the halves as of two packets) and then recombined to interfere. Meanwhile, each of the two packets progresses through a separate long cylindrical metal tube connected again to a generator and playing the role of the Faraday cage from

the previous example. We want the length of the packets to be much bigger than their wavelength and much smaller than the length of the cylinders at the same time. The generators on the pipes are turned on – making thus scalar (and generally non–equal) potentials $\varphi_1(t)$ and $\varphi_2(t)$ non-zero – only during a short time interval when both the packets are well inside one tube or the other, and turned off otherwise. The field does not penetrate far into the tubes from their edges, and there is no other external field or potential present in the system. This ensures that the electrons in both packets experience merely the corresponding time-dependent potential but no local electric field. However, a real physical effect in the form of a relative phase shift between the two packets will occur, as shown below.

When the generators are off (i.e. the potentials are zero), the wave function is a superposition of the wave functions of both packets, namely

$$\psi^0 = \psi_1^0 + \psi_2^0.$$

Turning the generators on and thus applying the potentials on the tubes causes them to behave as the individual Farraday cages in the previous example; this gives

$$\psi = \psi_1^0 e^{\imath S_1/\hbar} + \psi_2^0 e^{\imath S_2/\hbar}$$

where again

$$S_i = \int e\varphi_i \,\mathrm{d}t.$$

Evidently, the interference of the two beams depends on the phase difference $(S_1 - S_2)/\hbar$ determined solely by the potentials and thus a change in the interference pattern can be observed even without any influence of the fields.

Magnetic AB effect

We proceed to the second experiment; the setup is shown in Fig. 3.2. A closely wounded cylindrical solenoid with the center in the origin and oriented in the direction of the $z-$axis is introduced. The return magnetic flux is made to avoid the regions where the electrons are permitted. Again, an electron beam comes from the left, splits into two parts passing the solenoid from different sides without touching it, and reunites to form an interference pattern. Since there is no time dependence, neither making wave packets is necessary in this case.

By supplying an electric current to the solenoid, a stationary magnetic field H is created, enclosed completely within the solenoid. However, contrary to the field, the vector potential A cannot vanish everywhere outside the solenoid, since the path integral of A along any simple closed trajectory

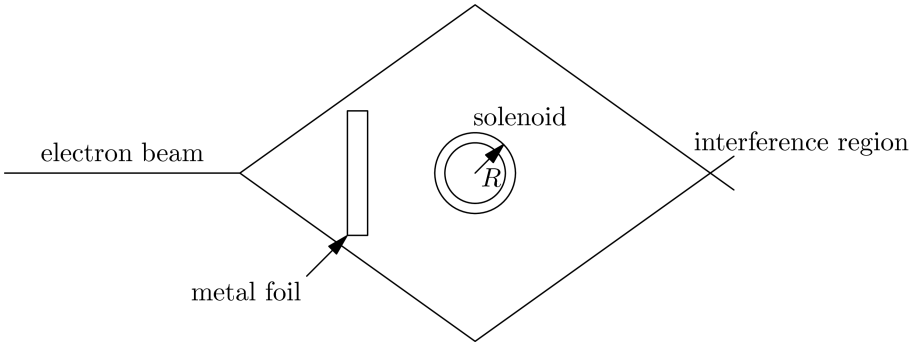

Figure 3.2: Magnetic AB effect

around the solenoid is constant and equal to the total magnetic flux ϕ inside it, i.e.

$$\int \mathrm{H}\,\mathrm{d}S = \oint A\,\mathrm{d}x = \phi.$$

The Hamiltonian of the system reads

$$H = \frac{1}{2m}\left(-i\hbar\nabla + \frac{e}{c}A\right)^2.$$

As with the electric type of effect, we can write the wave function as $\psi^0 = \psi_1^0 + \psi_2^0$ for the free case (i.e. when A = 0); here ψ_i^0 represent the beam halves on one or the other side of the solenoid.

Suppose that $A \neq 0$ now. If we had a simply connected region where $\mathrm{H} = \nabla \times A = 0$, an electron traveling along a path P would acquire a phase

$$S = \frac{e}{\hbar}\int_P \mathrm{A}\,\mathrm{d}x$$

and therefore the solution for the above Hamiltonian H would be $\psi = \psi^0 e^{-\imath S/\hbar}$. In our situation, the region is multiply connected and ψ is generally not single-valued, making it inadmissible as a solution. However, we can treat both beams independently since they lie in two distinct regions, each of them being simply connected, and use the above argument individually for each of them. Thus

$$\psi = \psi_1^0 e^{-\imath S/\hbar} + \psi_2^0 e^{-\imath S/\hbar}, \qquad S_i = \frac{e}{\hbar}\int_{P_i} A\,\mathrm{d}x$$

with P_i standing for paths of the first and the second beam, respectively.

The phase difference determining the interference then reads

$$\frac{1}{\hbar}\left(S_1 - S_2\right) = -\frac{e}{\hbar c}\oint A\,\mathrm{d}x = \frac{e}{\hbar c}\phi.$$

Evidently, it depends on the value of the flux only. Again, the effect occurs even though the particles do not experience the field.

The two types of the effect

As said, the AB effect is of dual nature, appearing in both its electric and magnetic variants. These two effects are however not different phenomena, but they are rather closely linked. We will describe now what separates and connects them.

What distinguishes the two variants (from a technical point of view) are the types of potentials and integrals involved. In the electric AB effect, scalar, time-dependent electric potentials play the crucial role. On the contrary, those appearing in the magnetic AB effect are vector, space-dependent magnetic potentials. The phase differences determining the interference patterns can be expressed as a time integral in the former variant and a loop time-independent integral in the latter, namely

$$\frac{1}{\hbar}\,(S_1 - S_2) = \begin{cases} \dfrac{e}{\hbar}\displaystyle\int (\varphi_1 - \varphi_2)\ \mathrm{d}t, & \text{(electric type)} \\ -\dfrac{e}{\hbar c}\displaystyle\oint A\,\mathrm{d}x & \text{(magnetic type)} \end{cases}$$

with integration around any closed curve around origin in the second case.

On the other hand, the above integrals show us a connection as well. They can be looked on as the components of the covariant product of two four-vectors, namely potential $A_\mu = (A, -\varphi/c)$ and space-time differential $\mathrm{dx}^\mu = (\mathrm{dx}, c\,\mathrm{dt})$. Here, c and x denote respectively the light velocity and the displacement vector, and $\varphi = \varphi_1 + \varphi_2$ is a total potential of the electric AB effect. This leads to a relativistic generalization of these integrals in the form

$$\frac{e}{\hbar}\oint \left(\varphi\,\mathrm{d}t - \frac{A}{c}\,\mathrm{d}x\right)$$

with the path of integration going over any closed curve in space-time and φ being evaluated in the center of the wave packet. So, if one started only with the electric AB effect, the described generalization would lead to a conlusion that the magnetic effect exists as well – in fact, this is exactly the argumentation used in [AB1].

The essence of the effect is the same for both variants, too. It lies in the exclusion of the fields from contact with the particles, creating thus a multiply connected space. This is clearly visible in the case of the magnetic type of effect, where the excluded region lies in between the two beam halves. For

the electric variant, the multiply connected region surrounding the excluded field has to be considered as a region in the space-time.

Finally, the magnetic AB effect can also be observed as an electric effect in a coordinate system where the incident electron is at rest (c.f. [K]). In [L1] it was shown that the invariant quantity to a Lorentz transformation can be given by an electromagnetic flux $\oint A_\mu \,\mathrm{d}x^\mu = \oint A \,\mathrm{d}x - \varphi \,\mathrm{d}t$.

Magnetic AB effect in detail

A general form of the "magnetic Aharonov-Bohm Hamiltonian", i.e. the Hamiltonian of the system with excluded magnetic field, reads

$$H = \frac{1}{2m}\left(-\imath\hbar\nabla + \frac{e}{c}(A_{AB} + A_0)\right)^2 - eV_0. \tag{3.1}$$

Here A_0 and V_0 denote some ordinary potentials, whose respective electromagnetic field may overlap with the domain of the electron, and A_{AB} is the potential due to the excluded stationary magnetic field. With $A_{AB} = 0$, the operator has the form

$$H_0 = \frac{1}{2m}\left(-\imath\hbar\nabla + \frac{e}{c}A_0\right)^2 - eV_0.$$

Let us denote ψ and ψ_0 the solutions of the corresponding Schrödinger equations for operators H and H_0.

The operators and their solution are formally related by the gauge transformation

$$U(x) = \exp\left(-\frac{\imath e}{\hbar c}\int_x A_{AB}\right) \tag{3.2}$$

where the path of integration is any closed curve going through the point x, and

$$H = UH_0U^{-1}, \qquad \psi = U\psi_0. \tag{3.3}$$

If they held true, equations (3.2) and (3.3) would imply that there is no observable effect of the excluded field on the electron, and thus H and H_0 would describe the same systems.

However, the relations are only formal so far. To form a real gauge transformation and to ensure that $\psi = U\psi_0$ is the unique solution of the Schrödinger equation for H, U must be a single-valued function independent of the path of integration in (3.2) for given x.

For a simply connected domain of the electron, it suffices that $\mathrm{H} = \nabla \times \mathrm{A_{AB}} = 0$ within it. Then the above conditions are fulfilled and there is no observable AB effect.

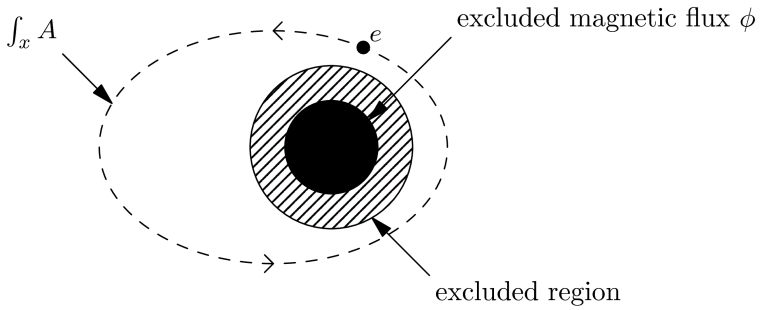

Figure 3.3: Excluded regions, excluded magnetic field

Let us suppose the domain is multiply connected, however. If the field is confined to an excluded region as in Fig. 3.3, then U is generally not single valued even if $\mathrm{H} = 0$ in the whole domain. Therefore U does not constitute a gauge transformation, the systems described by H and H_0 are different and the dynamics of the electron in the former system depends on the magnetic flux ϕ.

This dependence causes all observable phenomena to behave periodically. As said, the phase shift is gauge invariant and is determined by

$$\left(S_1 - S_2\right)/\hbar = -\frac{e}{\hbar c} \oint A_{AB}\,\mathrm{d}x = \frac{e}{\hbar c}\phi,$$

therefore the period is equal to London's unit $\phi_0 = 2\pi\hbar c/e$.

As a consequence, there is a special case when the AB effect vanishes even though there is an excluded field. It happens when the flux is an integer multiple of ϕ_0. Then integrating around the excluded field changes U by the factor $\exp(2n\pi\imath)$, keeping it single valued.

It is usual to define α, where

$$\alpha = -\frac{e\phi}{2\pi c\hbar}, \tag{3.4}$$

as a parameter of the AB effect. Due to the gauge symmetry mentioned above, which can be described as $A'_{AB} = A_{AB} + e^{e\imath\theta}, n \in \mathbb{N}, \theta \in [0, 2\pi]$ as well, one can always consider $\alpha \in (0, 1)$ without loss of generality. Analogously, the effect disappears for $\alpha \in \mathbb{N}$.

3.1.2 Significance of AB effect in quantum theory

The interpretation proposed by Aharonov and Bohm was not widely accepted after the publication of [AB1], with some papers even denying the very existence of the effect, and it was not until 1986 that the effect was experimentally

demonstrated in a manner satisfying its opponents and described in [TOM$^+$]. Nowadays, there is a widespread agreement about the significance of the effect. For a detailed historical review with a comprehensive list of references, see [OP] or the books [PT] and [H2].

History

At the beginning of 1960s, early attempts to demonstrate the effect experimentally were made. The very first one was conducted by Chambers ([C2]) using a tampered whisker in 1960, and followed by several others. Though the experiments showed the predicted interference shifts, Aharonov and Bohm stressed in their second paper in 1961 (cf.[AB2]) that they did not serve as an ideal confirmation, the issue being an insufficient separation of the effect of vector potentials from that of magnetic fields. Subsequently, special attention was paid to the detention of a pure potential effect in the experiment by Mölenstedt and Bayh in 1962 ([MB]). However, the level of suppression of the leakage field was still not perfect, leaving space for a possible alternative explanation of the interference patterns due to the fields, and denying the role of potentials.

Simultaneously with these experiments, theoretical discussion about the interpretation of the effect and about the actual significance of potentials started, with both supporting and disapproving arguments presented in papers. The dispute was further fueled by the introduction of the concept of non-integrable phase factor by Wu and Yang ([WY]); according to them, the AB effect demonstrated the gauge principle of electromagnetism. There were also attempts to interpret the effect in the classical framework as an interaction between the electron and the magnetic field.

Probably the most serious critics were Bocchieri and Loinger, who produced several articles questioning both theoretical and experimental results. In [BL] and subsequent papers, they claimed that the effect does not exist at all, being a purely mathematical construction, and that fields are the only relevant physical entities. They brought in a lot of arguments supporting their assertion. The most essential concerned a possibility to choose a gauge function so that the vector potential vanishes outside the solenoid, a possibility to replace the Schrödinger equation by a set of nonlinear differential equations containing only fields, the alleged nonexistence of the AB effect for bound state electrons scattering, as well as the nonexistence of the AB scattering. As for experiments, they claimed the interference pattern can be fully explained by leakage fields. Their work invoked quite a strong reaction with several articles advocating Bocchieri's and Loinger's conclusion, but with the majority of papers supporting those of Aharonov and Bohm.

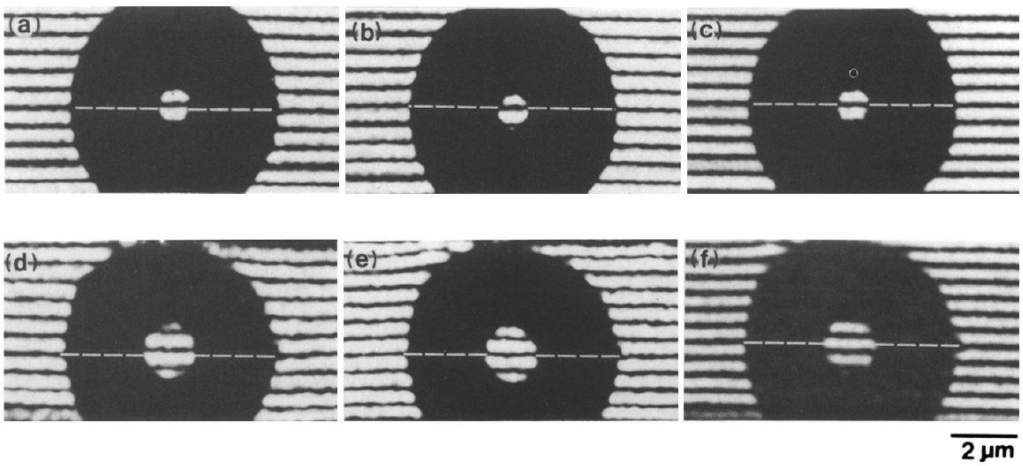

Figure 3.4: Interference patterns as published in [TOM$^+$]

Experimental proof of the effect

The final experiment was carried out in 1986 by Tonomura et al, resuming their previous attempts. The results were published in [TOM$^+$].

A tiny toroidal magnet of less than 10 μm was prepared and its surface covered by a metal layer of superconducting material, and further by a copper layer. This ensures that there is no possibility of electron penetration into the magnet, and, due to Meissner effect, the magnetic field cannot pass the layer and leak outside the toroid. In this setup, no overlap between the magnetic field and the electron beam is possible. (In fact, these effects were negligible rather than nonzero, with only 10^{-6} of the electron wave was estimated to reach the magnet through the shielding. Moreover, the leakage fields were measured using electron holography and only those toroid samples with nonmeasurable leakage were chosen and used.)

Two electron beams then were shined onto the toroid, one passing the hollow part of it, and the other going outside the toroid. Electron holograms were formed with a field-emission electron microscope, and the waves were recombined to form an interference pattern. The pattern was recorded as a hologram and optically reconstructed using two laser beams. The phase shift of size $2e\pi\phi/\hbar$ appeared with ϕ being the magnetic flux enclosed by the beams. This proved the existence of the effect. The interference patterns are depicted in Fig. 3.4.

As a by-product of the experiment, quantization of the flux was proven, with the interferograms changing abruptly when a superconducting critical temperature was passed.

3.2 The systems

In this part, we will provide the definitions of the systems we are interested in, including some formal operators describing them. We will also define some commonly used terms here.

After some general remarks in 3.2.1, we will start with the pure AB effect with no other influence, and its idealized version (in 3.2.2 and 3.2.3). Then a homogeneous magnetic field will be added into the system in 3.2.4. Finally, there will be some discussion concerning the choice of boundary conditions in 3.2.5.

3.2.1 General remarks

From now on, we will concentrate on the magnetic version of the phenomena. Thus, by the AB effect we will always mean the magnetic Aharonov-Bohm effect, unless stated otherwise.

For the sake of convenience, we will also introduce the natural units usual in mathematical literature, i.e. we will put $\hbar = e = m = c = 1$ from here on. There will be some few exceptions to the rule in Sections 3.3 and 3.5 where a review of the related research will be present – we will preserve the notation standards of the papers cited there.

We will consider spinless particles. Again, there will be exceptions in the review of the literature later on.

3.2.2 Pure AB effect

We will start with the AB effect with no other influence, i.e. when $V_0 = A_0 = 0$, and $A_{AB} \neq 0$ in (3.1). This system is sometimes titled "pure AB effect" and its formal Hamiltonian reads

$$H = (-\imath\nabla + A_{AB})^2 = -(\nabla + A_{AB}(\nabla))^2 \tag{3.5}$$

(we do not consider the self-adjointness of the operator here, thus no domain is specified).

Then, the solenoid is considered parallel with the $z-$axis, implying the magnetic field in the form

$$\mathrm{H}(x, y, z) = (0, 0, \mathrm{H}(r))$$

with $r^2 = x^2 + y^2$. In the general case, $H(r)$ must vanish for $r \geq R$, and in this region the magnetic potential can be taken in the form

$$A_{=}\frac{\imath\phi}{2\pi r^2}(-x_2 dx_1 + x_1 dx_2), \quad r^2 = x_1^2 + x_2^2.$$

where ϕ signifies the total flux. Then the parameter of the effect α is defined as in (3.4), namely

$$\alpha = -\frac{\phi}{2\pi},$$

with $\alpha \in (0, 1)$ without loss of generality.

3.2.3 Idealized AB effect

Shortly, the idealized AB effect is a combination of the pure AB effect with a singular potential.

In [AB1], the authors introduced an idealized setup with infinitely thin solenoid, i.e. in the limit where the diameter of the region with the magnetic field goes to zero while preserving the value of the total flux. This setup allows a particulary elegant treatment. It was later on referred to as the idealized AB effect.

The authors proved that the probability that the particle will traverse the magnetic field region tends to zero in the limit where the diameter of the solenoid goes to zero, too. They concluded that the beam can be shielded from the field by a barrier whose radius is infinitesimally small, and the wave function would remain intact.

Later on, the question of the appropriateness of the idealized setup was addressed, e.g. by [PTT] and [T1]. One could refer to an unclear sense of the separation of the flux from the electron domain when the radius of the excluded cylinder is zero. However, it was shown that putting the shield radius equal to some finite a and setting the solenoid radius to $a/2$, still leads to a flux-dependent cross section. Moreover, the wave function converges smoothly to the one computed in [AB1] when $a \to 0$. In [T1], the substitution of a toroidal solenoid for an infinite cylinder was discussed.

There are many ways the idealized AB effect (or the solenoid representing it) is referred to in the literature. The most common are "flux", "idealized solenoid", "singular AB effect" or "thread of a flux". In the two-dimensional cases, the point of intersection of the flux with the plane is called "vortex".

Mathematical description

The idealized AB effect can be formally described by the operator (3.5) with a singular potential added,

$$H = (-\imath\nabla + A_{AB})^2 - \lambda\,\delta(r) = -\left(\nabla + A_{AB}(\nabla)\right)^2 - \lambda\,\delta(r). \tag{3.6}$$

Here in the last term, λ denotes the coupling constant and δ is a symbolical expression of the singularity; its exact meaning is explained in Section 2.2.

Taking into consideration the translational symmetry with respect to z, it is possible to reduce the problem to two dimensions only. The Hamiltonian can then be rewritten in polar coordinates as

$$H_{AB} = -\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\imath\frac{\partial}{\partial\theta} - \alpha\right)^2 - \lambda\,\delta(r).$$

Here the term $\lambda\,\delta(r)$ has to be considered as a symbol standing for a singular potential in two dimensions, correspondingly.

The formal operator (3.6) may be interpreted as describing the combination of two interactions: 1. the magnetic interaction due to the pure AB effect, and 2. the contact interaction of the particle with the solenoid. (However, some other points of view are possible as well.)

There were several attempts to rigorously define the operator (3.6) and to handle the inweaved singularity; this is closely connected with the topic of Section 3.2.5, i.e. the problem of choosing boundary conditions.

The correct treatment of the operator uses the method based on the theory of self-adjoint extensions (cf. Section 2.2 for the two-dimensional case); the application of the method and the results will be discussed in Section 3.3.3.

3.2.4 AB effect and homogeneous magnetic field

The system we are interested in is composed of the idealized AB effect on the background of a homogeneous magnetic field.

The corresponding formal operator has a similar form as in (3.6), namely

$$H = (-\imath\nabla + A)^2 - \lambda\,\delta(r) = -\left(\nabla + A(\nabla)\right)^2 - \lambda\,\delta(r), \tag{3.7}$$

the difference being in the potentials. Here the vector potential A is the sum of two parts, $A = A_{\mathrm{hmf}} + A_{\mathrm{AB}}$, with the part A_{hmf} corresponding to the homogeneous magnetic field in the circular gauge,

$$A_{\mathrm{hmf}} = -\frac{\imath B}{2}(-x_2 dx_1 + x_1 dx_2),$$

and with the part A_{AB} corresponding to the idealised AB effect,

$$A_{\mathrm{AB}} = \frac{\imath\phi}{2\pi r^2}(-x_2 dx_1 + x_1 dx_2), \quad r^2 = x_1^2 + x_2^2.$$

Without loss of generality we may assume that $B > 0$. As in (3.4), we rescale the Aharonov-Bohm flux,

$$\alpha = -\frac{\phi}{2\pi},$$

to have a variable which expresses the number of flux quanta and, as usual, we make use of the gauge symmetry allowing us to assume that $\alpha \in (0, 1)$. We remind the case $\phi \in 2\pi\mathbb{Z}$ is excluded since it is gauge equivalent to the vanishing AB flux.

Once again, since the newly added magnetic field does not brake the rotational symmetry, the reduction to a two-dimensional problem remains feasible. This leads to the expression in polar coordinates in the form

$$H = -\frac{1}{r}\,\partial_r r \partial_r + \frac{1}{r^2}\left(m + \alpha + \frac{Br^2}{2}\right)^2 .$$

Since the magnetic field does not bring any new singularity, the issue of the proper definition of the singular potential is the same as with the idealized AB effect. The correct investigation of the problem is described in Section 3.4.

Perturbation of the homogeneous magnetic field

We will mention one possible physical interpretation of this system. Throughout this thesis, we stick to the following view: first, the idealized AB effect and its embedded singularity has to be dealt with. Only after that some other influence, in this case the magnetic field, can be added. However, it is possible to see it from a different perspective.

One can view the Hamiltonian as the simplest perturbation to the Landau operator or, in other words, regard the AB flux as the simplest magnetic perturbation of the homogeneous field. Thus, one can think about the system as of the simplest (even explicitly solvable) quantum system with inhomogeneous magnetic field; as is well known, other systems of this kind are very difficult to deal with.

3.2.5 Boundary conditions

Throughout the whole Chapter 3, there will be one area of special interest and importance to us, namely the boundary conditions.

With the magnetic type of the AB effect, there arises a question of behavior of the wave packet when it reaches the solenoid border (or better said, the border of the shield confining the solenoid), regardless of its diameter; this concerns both the hard-core and the idealized setups, i.e. cases where $R > 0$ and $R \to 0$, with R being the solenoid diameter.

We will consider the idealized setup here. In this case, the problem of boundary conditions can in fact be transformed to the problem of a correct definition of singular potentials, and of the Hamiltonians containing them.

One can view the definition of the operators from three equivalent angles: 1. treating the singularity included in the potential, 2. choosing the boundary conditions at the origin, 3. specifying the domains of the operators.

In [AB1], the condition of regularity was imposed on the electron wave, namely $\lim_{r\to 0}\psi(r,\theta) = 0$ in polar coordinates. It seemed to be a natural choice in agreement with the intuition, the idea being that the wave packet disappears when reaching the solenoid.

However, it was shown later on that this is not the most general admissible condition from the mathematical point of view ([AW], [dSG]), and that one can allow the wave function to be singular at the beginning. In this way, a class of properly defined Hamiltonians depending on the choice of boundary conditions and describing the system appears. Moreover, it shows that there are observable differences (changes in the spectrum, differential cross sections etc.) between the particular systems corresponding to different operators. Thus, with restriction to the regular boundary condition full physical description of the effect is not achieved.

Concerning the idealized AB effect, there are essentially three types of conditions used in the literature. Firstly, the mentioned regular condition used e.g. in [AB1] and [R3]. Secondly, conditions allowing singular behavior of the wave functions separately in p- and s-wave (i.e. in fixed sectors of angular momentum with $m = 0$ and $m = -1$), used e.g. in [GHKL], [GMS], and [MT]. And lastly, the most general conditions derived simultaneously by [DŠ] and [AT]. We will study these types of conditions in the following three parts 3.3.1, 3.3.2, and 3.3.3.

As to the case with the added magnetic field, the literature is sparser here. Hence, very few such illustrating examples can be found, the only ones being the condition $\psi(0) = 0$ used in [T2], and the regular condition in [C1]. The most general conditions are derived in [EŠV].

3.3 Preceding research

A brief review of literature follows, with the intention to show [EŠV] in its broader context of preceding work. Amongst the many papers published on the subject, only few were chosen, selected by two criteria.

Either, the articles are direct predecessors of [EŠV], and thus they consider a similar physical system. The goal is mainly to show the state of the art at the time of publication.

Or, the articles consider the topics from the similar viewpoint, and hence illustrate in practice the discussion from the previous part. Here the aim is to show the evolving approach to the question of boundary conditions and their

progressive generalization leading at the end to the broadest formulation of the problem as presented in [DŠ] and [EŠV].

Concerning the second type of articles, a word of explanation is in order. The systems with only the AB effect on one side and those with the magnetic field included on the other are essentially different concerning the results, e.g. when it comes to the subject of spectra. While the former have purely continuous spectra and only a small number of bound states (and thus the scattering occurs), the latter have pure point spectra. Thus, we will state here some results which are not connected to the outcome of [EŠV], e.g. scattering amplitudes, cross sections etc. Rather then the results themselves how they were obtained and how they were influenced by the respective definition of the operators is of more interest to us.

For the same reasons the two physical situations, i.e. the AB effect with and without the homogeneous magnetic field, are covered in the same section. The approach to both systems is analogous, and the similarities in this attitude are more important than the differences concerning the outputs in our view.

The key to division of this section are the boundary conditions. The first three parts are devoted to papers using the three types of them as mentioned in Section 3.2.5, being in turn the regular condition, the s- and p-wave approach, and the most general boundary conditions. In all these parts, the idealized AB effect is treated. Then the literature about the AB effect and the homogeneous magnetic field follows in Section 3.2.4.

3.3.1 Regular boundary condition

We start with the results of the original article [AB1] and with one of the most well-known study of the idealized AB effect [R3]. In both of them, the most simple boundary condition – i.e. the regular one – is used.

Aharonov and Bohm, 1959

The first results were posted in the same article where the idea of the effect was introduced, in [AB1]. Therein, authors study the problem of the scattering of an electron beam by a magnetic field in the idealized setup, and obtain an exact solution.

The formula for the scattering cross section

$$\sigma = \frac{\sin^2 \pi\alpha}{2\pi} \frac{1}{\cos^2(\theta/2)}$$

is computed. Then the stationary scattering method is used, and the asymptotic behavior of the wave function is found to be

$$\psi \sim e^{\imath kx+\imath\alpha\theta} + \frac{e^{\imath kr}}{(2\pi\imath kr)^{1/2}} \sin\pi\alpha \frac{e^{-\imath\theta/2}}{\cos(\theta/2)},$$

where the first part denotes the incident wave, while the second corresponds to the scattered wave. That gives the scattering amplitude in the form

$$\frac{1}{\sqrt{2\pi\imath r'}} \sin\pi\alpha \frac{1}{\cos(\theta/2)}. \tag{3.8}$$

According to the general prediction, it follows from these expressions that the effect vanishes for $\alpha = n$, and that the cross section reaches its maximum for $\alpha = n + 1/2$.

Ruijsenaars, 1983

In [R3], a detailed analysis of the scattering problem is carried out. Both idealized and hard-core cases are studied, and for each of them, two slightly different Hamiltonians are considered, giving thus four different operators. Then, scattering in all these cases is investigated using the time-dependent theory based on the wave operators, as well as the time-independent approach.

Since the hard-core case is studied mainly for the purpose of experimental testing, only some brief remarks will be made to it. The idealized case will be mentioned in more detail now. The starting point in [R3] is the formal operator

$$H_{AB} = -\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\imath\frac{\partial}{\partial\theta} - \alpha\right)^2,$$

from which the two Hamiltonians are derived, using two different approaches. In the first approach, the operator is decomposed to the sum of operators acting on angular momentum subspaces, reading

$$H_1 = \sum_{m\in\mathbb{Z}}^{\oplus} H_{m+\alpha}\,,$$
$$H_{m+\alpha} = -\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{(m+\alpha)^2}{r^2}.$$

In the other approach, the operator is written as

$$H_2 = e^{-i\alpha\theta}\left(-\partial_r^2 - \frac{1}{r}\partial_r - \frac{1}{r^2}\partial_\theta^2\right)e^{i\alpha\theta},$$

thus $H_2 = e^{-i\alpha\theta} H_0 e^{i\alpha\theta}$, where H_0 is the operator for the free case with $\alpha = 0$. These operators differ in the interpretation of the expression $\imath\partial_\theta - \alpha$, and they have different boundary condition for functions φ in their domain, namely

$$\lim_{\theta\uparrow\pi} \varphi(\theta) = \lim_{\theta\downarrow-\pi} \varphi(\theta)$$

for the former and

$$\lim_{\theta\uparrow\pi} \varphi(\theta) = e^{-2\imath\alpha\pi} \lim_{\theta\downarrow-\pi} \varphi(\theta)$$

for the latter operator. One can see that even the mathematical definition alone was ambiguous.

Then the analysis is carried out. Among other results, the S-matrix for H_1 is obtained, as well as the differential cross section in the form

$$\frac{d\sigma}{d\theta} = \frac{1}{2\pi k} \frac{\sin^2 \pi\alpha}{\sin^2 \theta/2};$$

also the differential cross section for the hard-core case converges to the same result for $kr \to 0$.

In Appendix, the boundary conditions we are interested in are discussed. The operator H_1 is considered, and in order to define it rigorously, the self-adjointness of its corresponding restrictions $H_{m+\alpha}$ is investigated. While the operators with $|m + \alpha| \geq 1$ are concluded to be essentially self-adjoint, the possibility of having one-parameter family of s.a. extensions is stated for $|m+\alpha| < 1$, and the possibility of having "unorthodox" boundary conditions is admitted at several places in the text. However, the Dirichlet boundary condition is imposed in the end, ruling out other s.a. extensions.

3.3.2 The p- and s- waves

The conclusion that the regular boundary condition was too strong a requirement was published several times, see the discussion in 3.2.5. As a reaction to that, the articles [GHKL], [GMS], [MT] appeared, trying to tackle the problem. In the papers, singular behavior of the wave functions is allowed, as long as they fulfill some specified boundary conditions.

However, the proposed solutions are not the most general ones since in all the papers the decompositions to fixed angular momentum sectors is deployed first, and only after that the self-adjoint extensions are being looked for in each sector separately. Correspondingly, the boundary conditions are confined to those sectors as well. The deficiency indices are found to be (1,1) for $m = 0$ and $m = -1$, i.e. for the s- and p-waves, leading to a 2-parameter family of self-adjoint extensions while the correct approach gives

4 parameters. All the found self-adjoint operators commute with the angular momentum operator (which otherwise is not a general feature), and the possibility of coupling between the sectors is omitted.

Manuel and Tarrach, 1991

In this paper, the authors work with the concept of anyons – the particles in the two-dimensional space whose wavefunctions acquire a phase different from ± 1 when performing a 2π rotation, being the generalization of boson and fermion ideas. The concept of contact interactions due to a $\delta-$potential is used as well, and the need of imposing boundary conditions to ensure the self-adjointness of the system Hamiltonian is discussed. The contact interactions are linked to the AB effect, the value of the flux determining the strength of the interactions.

Here, one starts with the formal operator

$$H = -\frac{\hbar^2}{2M}\left(\partial_r^2 + \frac{1}{r}\partial_r + \frac{1}{r^2}\partial_\varphi^2\right) + V(r)$$

and a phase change $\exp(\imath\theta)$ under rotation of 2π, i.e.

$$\psi_\theta(r, \varphi + 2\pi) = \exp(\imath\theta)\psi_\theta(r, \varphi),$$

with $\theta \in [0, 2\pi]$ counting the windings around the origin. Then magnetic flux Φ is introduced at the origin, and the particle is given an electric charge q (with $q\Phi/\hbar c = -\theta$) in the exchange for the multivaluedness of the wavefunction, leading to the gauge transformation

$$\psi(r, \varphi) = \exp(-\imath\theta\varphi/2\pi)\psi_\theta(r, \varphi) = \psi(r, \varphi + 2\pi),$$

and to the corresponding operator

$$H_\theta = -\frac{\hbar^2}{2M}\left(\partial_r^2 + \frac{1}{r}\partial_r + \frac{1}{r^2}\left(\partial_\varphi + \imath\frac{\theta}{2\pi}\right)^2\right) + V(r).$$

The operator is decomposed using the separation of variables, giving the equation in r in the form

$$\left(-\frac{\hbar^2}{2M}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r} - \frac{\nu^2}{r^2}\right) + V(r)\right)\phi(r) = E\phi(r) \tag{3.9}$$

with $\nu = |m + \theta/2\pi|$, and $m \in \mathbb{Z}$.

The boundary conditions are then studied. For $V(r) = 0$, the solution ϕ of (3.9) is regularized by $u(r) = r^\nu\phi(r)$ so that the regularity condition

$u(0) = 0$ corresponds to the free solution with no flux present. To assure the self-adjointness of the operators, the boundary condition

$$u(0) \pm R^{2\nu} \frac{\mathrm{d}u(r)}{\mathrm{d}r^{2\nu}}\bigg|_{r=0} = 0 \tag{3.10}$$

is imposed at $r = 0$, with some arbitrary R. The results for zero and negative values of m are studied. For the s-waves, the scattering is stated to be present for $\nu < 1$, and the phase shift computed. For each sector $m < 0$, one eigenvalue is found under the condition $\nu < 1$, again.

Here, the regularity condition $u(0) = 0$ is just a special limiting case of the general boundary condition (3.10). However, both of these conditions are applied only in the fixed angular momentum sector, not to the functions from the domain of the operator H_θ.

Giaccconi et al, 1996

The paper [GMS] was aimed at dealing with two issues which the authors considered not being treated correctly so far – namely, the evaluation of the scattering amplitude in the forward and backward direction, and the problem of the choice of the boundary conditions.

According to the authors, there were two ways of computing the scattering amplitude in the literature. In the first approach used by [AB1] and [BCL$^+$], the amplitude was derived directly from the asymptotic behavior of the stationary scattering states, however losing its meaning in the forward and backward direction since the asymptotic formula holds true only for $|\varphi \neq l\pi|, l \in \mathbb{Z}$, and φ being the polar coordinates angle. In the second one, used e.g. by [R3], it was computed from the sum of the partial amplitudes, causing the problem with the correct definition of the arising delta functions.

In this article, a different method is introduced. It starts with the scattering integral equation, and involves the use of the concept of adiabatic switching of the interaction from the perturbation theory, as well as the use of the analytic continuation of the scattering amplitude. To this aim, the stationary scattering wave function ψ_k is split into three parts – the regular part, and the s- and p-waves, with the angular momentum $n = 0$ and $n = 1$, respectively. The scattering amplitude according to the regular part,

$$F_k(\varphi) = \frac{1}{\sqrt{2\pi\imath k}} \left(1 - \cos\pi\alpha - e^{-\imath\varphi}\left(e^{-\imath\pi\alpha} - 1\right) - \sin\pi\alpha \cot\frac{\varphi}{2}\right) \tag{3.11}$$

with $\varphi \neq 2l\pi$, is then computed, being exactly equal to the appropriate part of the amplitude (3.8) obtained in [AB1]. In the forward direction the

following expression holds true,

$$F_k(\varphi = 2l\pi) = \frac{1}{\sqrt{2\pi\imath k}} \left(2(1-\cos\pi\alpha) + \imath(1+\alpha)\sin\pi\alpha\right),$$

and the incoming wave is a standard plane wave containing no delta functions.

As for the singular part, it is stated that the condition of regularity at the origin is too strong for s- and p-waves, and that even with singularities one can assure the self-adjointness of the Hamiltonian. The deficiency indices are computed to be $(1,1)$ for each angular momentum sector, and the most general asymptotic behavior of the wave function at the origin is obtained as

$$\psi(r) \sim \sum_{n=0,1} c_n r^{\gamma(n)};$$

for small r, with c_n being $r-$independent and $\gamma_n \in (0,1)$. The exact form of the s- and p-waves is derived using this boundary condition. Then, it is concluded that for every couple of parameters corresponding to two s.a. extensions (one in each sector) there exist two negative eigenvalues, E_0 and E_1, and their normalized eigenfunctions orthogonal to the scattering states are found.

In order to regularize the s- and p- scattering wave functions, limits $E_n \to -\infty$ are considered. The bound states disappear and the regular scattering wave functions form the complete orthonormal set that diagonalizes the Hamiltonian. The scattering amplitudes for $n = 0, 1$ are obtained as

$$\lim_{E_0\to-\infty} f_0(k; E_0) = \frac{1}{\sqrt{2\pi\imath k}} \left(e^{\imath\pi\alpha} - 1\right),$$
$$\lim_{E_1\to-\infty} f_1(k; \varphi; E_1) = \frac{e^{-\imath\varphi}}{\sqrt{2\pi\imath k}} \left(e^{-\imath\pi\alpha} - 1\right);$$

combined with (3.11) they give the formula 3.8. Moreover, the phase shifts corresponding to the AB effect as well as to the singular potentials are calculated, correcting the formulas given in [MT].

Finally, a brief discussion of the results follows. Taking the limits $E_n \to 0$ leads to purely singular eigenfunctions. The case of the vanishing AB effect when $\alpha \to 0$ is studied and corresponding scattering amplitudes for the s- and p- waves are found, with only the s-wave having a singular part, while the p-wave not being influenced by the δ potential.

3.3.3 Generalized boundary conditions

We will now focus on two simultaneously written articles, namely [DŠ] and [AT]. We describe them more in detail as they were the first to provide

a rigorous and mathematically correct treatment of the operators describing the idealized AB effect. Especially the paper [DŠ] will be of great importance to us, because it will be closely followed in 3.4, when the magnetic field will be added into the system.

Correct treatment of the Hamiltonians

In [DŠ] and [AT], the idealized AB setup is considered. Both papers use the method developed in [AGHKH2] and described in detail in Section 2.2. They define properly the Hamiltonians involving the singular AB potentials by the means of the theory of self-adjoint extensions.

In the papers, one starts with the operator

$$H = -\left(\nabla + A_{AB}(\nabla)\right)^2,$$

with the domain of smooth functions vanishing at the origin, $D(H) = C_0^\infty(\mathbb{R}^2 \setminus \{0\})$. Then its closure $\widetilde{H}$ is introduced, and all possible self-adjoint extensions of $\widetilde{H}$ are found.

For that, one needs to solve the eigenvalue problem

$$\widetilde{H}^* f = \pm \imath f$$

for the adjoint operator $\widetilde{H}^* = -\left(\nabla + A_{AB}(\nabla)\right)^2$ with domain

$$D(\widetilde{H}^*) = \left\{ \psi \in L^2(\mathbb{R}^2) \cap H^{2,2}_{loc}(\mathbb{R}^2 \setminus \{0\}) \;\middle|\; \left(\nabla + A_{AB}(\nabla)\right)^2 \psi \in L^2(\mathbb{R}^2) \right\}.$$

Then the decomposition of the Hilbert space is deployed,

$$L^2(\mathbb{R}^2, \mathrm{d}^2x) = \sum_{m\in\mathbb{Z}}^{\oplus} L^2(\mathbb{R}_+, r\,\mathrm{d}r) \otimes \mathbb{C}\, e^{\imath m\theta},$$

with the Hamiltonian decomposing accordingly as

$$\widetilde{H}^* = \sum_{m\in\mathbb{Z}}^{\oplus} (\widetilde{H}^*)_m. \tag{3.12}$$

The eigenvalue problem is then solved in every sector of the angular momentum separately, giving two L^2-integrable solutions

$$\begin{aligned}
f_\imath^{-1}(r,\theta) &= N_1 H^{(1)}_{1-\alpha}(kr) e^{-\imath\theta}, \\
f_{-\imath}^{-1}(r,\theta) &= N_1 e^{\imath\pi(1-\alpha)/2} H^{(1)}_{1-\alpha}(kr) e^{-\imath\theta}, \\
f_\imath^{0}(r,\theta) &= N_2 H^{(1)}_{\alpha}(kr) \\
f_\imath^{0}(r,\theta) &= N_2 e^{\imath\pi\alpha/2} H^{(1)}_{\alpha}(kr)
\end{aligned}$$

for each of the angular momentum sectors $m = -1$ and $m = 0$. Here $H^{(1)}_{|m+\alpha|}$ denotes the Henkel function and N_1, N_2 are some normalization constants. It follows that the operators $\widetilde{H}^*_m$ are self-adjoint for $m \neq -1, 0$, while $\widetilde{H}^*_{-1}$ and $\widetilde{H}^*_0$ have deficiency indices (1,1).

Thus the deficiency indices of $\widetilde{H}$ turn out to be $(2, 2)$. In comparison with the case of point interaction only, where for the free Laplacian the deficiency indices are found to be equal to $(1, 1)$, it shows that one cannot simply take a superposition of the results for the AB effect and the point interaction alone.

The self-adjoint extensions are in one-to-one correspondence with 2×2 unitary matrices, depending thus on four real parameters. Altogether, the Hamiltonians describing the system form a five-parameter family. Here, the last parameter corresponds to the parameter α of the AB effect, denoting its flux.

The domain of $\widetilde{H}$ is found as a consequence of the process, being

$$D(\widetilde{H}) = \left\{ \psi \in D(\widetilde{H}^*) \,\middle|\, \left\langle \psi \widetilde{H}^*, \varphi \right\rangle = \left\langle \widetilde{H}^* \psi, \varphi \right\rangle, \forall \varphi \in \mathcal{N}_\imath + \mathcal{N}_{-\imath} \right\} \quad (3.13)$$

where $\mathcal{N}_\imath$, $\mathcal{N}_{-\imath}$ denote the deficiency subspaces. Due to the decomposition (3.12), the functions $f \in D(\widetilde{H})$ decompose correspondingly and it is possible to write $f(r, \theta) = \sum_m g_m(r)(2\pi)^{-1/2} e^{\imath m\theta}$. Then the condition in (3.13) is equivalent to the condition on g_m in sectors $m = -1, 0$ in the form

$$\lim_{r \to 0_+} rW(g_m, h_\pm)_r = 0$$

where $h_\pm(r) = H^{(1)}_{|m+\alpha|}(\sqrt{\pm\imath} r)$ with $\mathrm{Im}\sqrt{\pm\imath} > 0$, and W denotes the Wronskian, $W(g, h)_r = \overline{g(r)} h'(r) - \overline{g'(r)} h(r)$.

The self-adjoint extensions H^U are expressed by means of unitary operators $U : \mathcal{N}_\imath \to \mathcal{N}_{-\imath}$ in the form

$$H^U u = \widetilde{H} v + \imath f_+ - \imath U f_+ \quad (3.14)$$

with

$$D(H^U) = \left\{ u \in L^2(\mathbb{R}^2) \mid u = v + f_+ + U f_+, v \in D(\widetilde{H}), f_+ \in \mathcal{N}_\imath \right\}$$

Then $\psi_+ = c_0 f^0_\imath + c_{-1} f^{-1}_\imath$ with constants $c_0, c_{-1} \in \mathbb{C}$, and $U\psi_+ = \tilde{c}_0 f^0_{-\imath} + \tilde{c}_{-1} f^{-1}_{-\imath}$ with $\tilde{c}_j = \sum_{l=0,-1} \tilde{U}_{jl} c_l$, $j = 0, -1$. The unitary matrix $\widetilde{U} \in U(2)$ can be represented as

$$\widetilde{U} = e^{\imath\eta} \begin{pmatrix} a & -\overline{b} \\ b & \overline{a} \end{pmatrix}, \qquad |a|^2 + |b|^2 = 1.$$

Several special cases are then discussed.

The choice $\widetilde{U} = -1$ corresponds to the Hamiltonian of the pure idealized AB effect with the regular condition studied in [AB1]. In this case the functions from the domain vanish at the origin. There is no point interaction and the only parameter of the Hamiltonian is the one corresponding to the AB effect, the magnetic flux α.

If $b = 0$ then $a = e^{\imath\tau}$ for some τ, and the extensions are characterized by parameters η and τ. Then the point interaction acts in the two sectors $m = -1, 0$ separately, and this leads to the case studied by [GHKL], [GMS], and [MT], i.e. to the stand-alone boundary conditions for the s- and p-waves. In general form, however, the coupling between the two sectors is realized.

The choice $\eta = \pi + \tau$, resp. $\eta = \pi - \tau$ eliminates the point interaction in the sector $m = -1$, resp. $m = 0$.

Having diagonal $\widetilde{U}$ means that the extension preserves the angular momentum.

In general, H^U is not rotationally invariant, and therefore the angular momentum is not a constant of motion.

Resolvents, spectrum and scattering

In both papers, the formulas for resolvent of arbitrary self-adjoint extension are found by the means of the Krein's method, using the known resolvent for the AB Hamiltonian of [AB1] denoted by H^{AB}, and a constructed base of the deficiency indices.

The spectrum is studied as well, taking advantage od the knowledge of the resolvent $R^U = (H^U - z)^{-1}$, as well as the fact that it is a rank two perturbation of the resolvent of $\widetilde{H}$. It is concluded that

$$\sigma(H^U) = \sigma_{ac}(H^{AB}) = [0, +\infty), \qquad \sigma_s(H^U) = \emptyset,$$

and that at most two eigenvalues (with always negative value) can emerge.

In [DŠ], an analysis of the point spectrum is carried out, and the conditions for having zero, one, and two eigenvalues were found depending on the boundary conditions. The eigenvectors in the form of a certain linear combination of function from deficiency spaces are found.

As for the scattering, a complete normalized basis of generalized eigenvectors is found. Consequently, the existence and completeness of the wave operators $W_\pm = \lim_{r\to\pm\infty} e^{\imath tH} e^{-\imath tH_0}$ is proven. In [AT], the scattering ampli-

tude is computed in the form

$$\begin{aligned} f_\alpha^U(k,\theta,\phi) = f_\alpha^{AB}(k,\theta,\phi) \\ + 4\sqrt{\frac{2i\pi}{k}}\,\cos\left(\frac{\pi}{2}\alpha\right)\,p_{00}(k)\,(-k^2)^\alpha \\ - 2\sqrt{\frac{2\pi}{ik}}\,\sqrt{2\,\sin(\pi\alpha)}\,e^{-i\pi(1-2\alpha)}\,p_{-10}(k)\,k\,e^{i\theta} \\ + 2\sqrt{\frac{2\pi}{ik}}\,\sqrt{2\,\sin(\pi\alpha)}\,e^{i\pi(1-2\alpha)}\,p_{0-1}(k)\,k\,e^{-i\phi} \\ - 4\sqrt{\frac{2i\pi}{k}}\,\sin\left(\frac{\pi}{2}\alpha\right)\,p_{-1-1}(k)\,(-k^2)^{1-\alpha}e^{-i(\phi-\theta)} \end{aligned}$$

adding to the well known formula of scattering amplitude f^{AB} associated to H^{AB} four new terms, depending on parameters of the point interaction p_{ij}. In [DŠ], the explicit expressions for the wave operators and the scattering operator $S = (W_+)^* W_-$ are computed.

Boundary conditions

Since the formulation of the Hamiltonians given in (3.14) is rather abstract, a simpler characterization of the operators is derived in [DŠ]. Every self-adjoint extension is described explicitly by some rigorously defined boundary conditions.

The asymptotic behavior of the radial parts of the functions from operators domains is studied, and four linear functionals corresponding to the two leading terms in sectors $m = -1, 0$ are introduced, denoted by Φ_l^m with $m, l = 1, 2$. The singular part of any $\psi \in D(H^U)$ is written by their virtue, as well as the explicit boundary conditions characterizing $D(H^U)$ in the dependence on U.

This formula is developed further, and the simplest form of boundary condition is derived from it. The Hamiltonians are parameterized by a matrix Λ in the form

$$\Lambda = \begin{pmatrix} u & \alpha\overline{w} \\ (1-\alpha)w & v \end{pmatrix}, \quad u, v \in \mathbb{R},\ w \in \mathbb{C},$$

and the relation between U and Λ is established. The requirement then reads: $\psi \in D(\overline{H}^*)$ lies in $D(H^\Lambda)$ if and only if

$$\begin{pmatrix} \Phi_1^1(\psi) \\ \Phi_1^2(\psi) \end{pmatrix} = \Lambda \begin{pmatrix} \Phi_2^1(\psi) \\ \Phi_2^2(\psi) \end{pmatrix}.$$

This technique is closely followed by [EŠV], and its application on the case with the magnetic field is described in 3.4.4.

3.3.4 Systems with the AB effect and magnetic field

The literature devoted to these systems is not as extensive as in the case of the pure AB effect. Thus, compared to previous three sections focused on different attitudes towards the definition of AB Hamiltonian, we do not divide the articles into groups, as this section serves mainly as a review of the papers published on the subject.

However, an interesting analogy with the previous discussion for the pure AB effect can be found, concerning the choice of the boundary conditions. There is an exceptional case in [T2] where the requirement $\psi(0) = 0$ is imposed. Then, the regular boundary condition is used in article [C1], while in [FP] the separate s- and p-waves approach is followed. None of them thus leads to the most general results. The situation is different with the papers [HO] and [N] – they treat the more general problem with more solenoids and their aim is distinct, hence the discussion about boundary conditions is not relevant in this case.

Thienel, 2000

The same situation as described in 3.2.4, with the exception of using a spin 1/2 particle, is studied in [T2]. The Hamiltonian (3.7) therefore reads

$$H = \frac{1}{2M}\left(p + \frac{|e|}{c}A\right)^2 + \frac{|e|\hbar}{Mc}B_z S_z.$$

The main goal of the article is to solve the eigenvalue problem.

The author uses two approaches to the subject and tries to prove that they do not lead to the right results. Consequently, a new method is introduced to remove the problems.

The first, "direct" approach tries to solve the eigenvalue problem with taking the δ-distributions into account. The magnetic field is taken as $B_z(r) = B + \alpha\Phi\delta^2(r)$, where $B > 0$ and $\alpha\Phi$ denote the flux of the singular tube, with $\alpha \in \mathbb{R}$ and $\Phi = 2\pi\hbar c/|e|$. That corresponds to the vector potential $A(x, y) = (Br/2 + \alpha\Phi/2\pi r)e_\varphi$ with the polar coordinates r, φ, leading to the Hamiltonian

$$\begin{aligned} H = -\frac{1}{4r}\,\partial_r r \partial_r - \frac{1}{4r^2}\left(\partial_\varphi + i\alpha\right)^2 - \frac{i}{2}\left(\partial_\varphi + i\alpha\right) + \\ + \frac{1}{4}\,r^2 + \left(1 + \frac{\alpha}{2r}\delta(r)\right) S_z \end{aligned} \tag{3.15}$$

The eigenvalue problem is handled using the commutativity of H_α with Ł$_z$ and S_z, and the separation of variables. In the following discussion, the

condition $\psi(0) = 0$ is imposed on solutions ψ. This, together with the requirement that each superpartner of any solution must be a solution as well, leads to a set of eigenvalues that, after being compared with the solutions of the case with no flux, is declared insufficient.

The second approach is based on taking a limit of systems with cylindrical flux tubes with finite radius R, with $R \to 0$. Inside the tube, another homogeneous field perpendicular to the plane is considered. The eigenvalue equation is solved with conditions imposed on the solutions, namely that it must be regular at the origin and vanish at infinity. Again, the solution set is stated to be unsatisfactorily small.

Then the new method is suggested. Instead of taking a limit of well defined systems, the idea is to take a limit of some abstract entities, where only the limiting system would be interpreted by the means of quantum mechanics. To this end, all the necessary concepts as scalar product, zero vector, probability density etc. have to be defined as a limit $R \to 0$ of the corresponding quantities. This relates to the boundary condition at the border of the tube in the form

$$\lim_{\tilde{R}\to 0} \left(\psi_{E',\sigma,m}(\tilde{R})\tilde{R}\frac{\partial}{\partial\tilde{r}}\psi^{\mathrm{in}}_{E,\sigma,m}(\tilde{r})\bigg|_{\tilde{r}=\tilde{R}} - \psi_{E',\sigma,m}(\tilde{R})\tilde{R}\,\frac{\partial}{\partial\tilde{r}}\psi^{\mathrm{out}}_{E,\sigma,m}(\tilde{r})\bigg|_{\tilde{r}=\tilde{R}} \right) = 0$$

as well. After the analysis of the boundary condition and some supersymmetry requirements, the eigenvalues are found. However, compared to the correct results, some eigenvalues are missing, leading thus to the conclusion that the corresponding eigenfunctions do not form a complete basis of the space.

Then some other issues are briefly discussed. The first one is the perturbation theory and the possibility to obtain the eigenvalues for any α from the exact knowledge of the system for some α_0. Then the subject of index theorems determining the difference between the number of eigenstates corresponding to different values of spin, as well as a discussion about symmetry breaking follows. Finally, the eigenvalue problem for the pure AB effect with $B = 0$ is handled, leading again to an uncomplete spectrum.

Shortly, only the standard extension is considered, even with controversy.

Cavalcanti, 2000

The article [C1] arose as a reaction to [T2], disagreeing with its claim that it is not possible to solve the eigenvalue problem either using the δ-distribution or treating the singular flux as the limit of cylindrical tubes. The author stated that both methods work well, assuming they are used properly.

First, starting with (3.15) and solving the eigenvalues equation, it is incorrect according to [C1] to require the solutions to vanish at the origin, i.e. to demand $\psi(0) = 0$. Instead, it must only hold true that $\lim_{r\to 0}\psi(r) = 0$ in compliance with [H1] and [G], who studied the case of the idealized AB effect without the magnetic field as a limiting case of finite size fluxes. This explains the problem with the vanished eigenvalues of [T2].

For $\alpha > 0$, the energies are computed to be

$$E_{n,m,1/2} = n + 1 + \frac{1}{2}\left(|m+\alpha| + m + \alpha\right), \quad n \in \mathbb{N}, m \in \mathbb{Z}$$

in concordance with results of [EŠV], and two superpartner eigenstates with the same energy and opposite spin are found. For $\alpha < 0$, the eigenvalues read

$$E_{n,m,-1/2} = n + \frac{1}{2}\left(|m+\alpha| + m + \alpha\right), \quad n \in \mathbb{N}, m \in \mathbb{Z}$$

with zero modes being those with $n = 0$ and $m + \alpha \leq 0$.

Finally, one can arrive at the same results using the limiting finite diameter approach. According to the author, wrong conclusion of [T2] was due to overlooked solutions of some particular equation.

Falomir and Pisani, 2000

The article [FP] considers the Dirac electron in two dimensions in the presence of a homogeneous magnetic field and one AB vertex localized at the origin. The need to use the Neumann's theory of deficiency indices and to construct the self-adjoint extensions is discussed thoroughly.

One starts with the Dirac operator H and then its commutation with the angular momentum operator is exploited, leading to operators H_m (the restrictions of H to each subspace corresponding to angular momentum m) in the form

$$H_m = \begin{pmatrix} m & \imath\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{1-m+\alpha}{r} - r\right) \\ \imath\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{m+\alpha}{r} + r\right) & -m \end{pmatrix}$$

acting on two-component functions $\psi(r)$. The domain of H_m is restricted to $D(H_m) = C_0^\infty(\mathbb{R}^+)$ so that it is symmetric, and the deficiency subspaces are found, with its bases denoted by ψ_m^+ and ψ_m^-. The operators H_m are discovered to be essentially self-adjoint except for $m = 0, -1$, where the deficiency indices are $(1, 1)$. The self-adjoint extensions depending on a parameter γ are constructed in both sectors, and the boundary conditions for the functions $\psi = (\phi, \xi)^T \in D(H_m)$ are derived as

$$\lim_{r\to 0_+} r\left(\phi\xi^\gamma - \xi\phi^\gamma\right) = 0,$$

where ϕ^γ and ξ^γ are components of $\psi^\gamma = \psi^+ + e^{\imath\gamma}\psi^-$.

The spectra of the self-adjoint extensions H_m^γ and of the other operators H_m with $m \neq 0, -1$ are investigated afterwards. The eigenvalues are stated to be

$$\lambda = \pm 2\sqrt{m^2/4 + \alpha + N}, \quad N \in \mathbb{N}, N \geq -l$$

for $m - \alpha > 1$, and

$$\lambda = \pm 2\sqrt{m^2/4 + N}, \quad N \in \mathbb{N}$$

for $m - \alpha < 0$. Moreover, the closure of H_m is studied, with the result that its corresponding boundary condition is the regular one.

In other words, this means that the extensions are considered merely in the individual sectors, as well as their respective boundary conditions, not on the level of operator H. This is the same approach as used in [GHKL], [GMS], and [MT] in the case of the pure AB effect. Again, coupling of the sectors is not allowed, leading to the same consequences discussed in 3.3.2.

System with many solenoids

The system investigated in [HO] is similar to ours. Namely, it consists of a charged particle with spin 1/2 in a two-dimensional magnetic field with two components: a magnetic field with bounded support (not necessarily homogeneous), and a "strongly singular magnetic field". The latter one is defined as $B_0(\cdot) = \sum_j \gamma^j \delta(\cdot - a_j)$, and is located in points a_j, the coefficients γ_j denoting the fluxes.

The aim is distinct, however – the authors investigate the dimension of the kernel of the Dirac-Weyl operator and consider the validity of Aharonov-Casher Theorem in this case (cf. [AC]), stating that the dimension of the kernel depends on the total flux $\Phi = \int_{\mathbb{R}^2} B dxdy$ only. They found out that in this case, the dimension depends on all the individual fluxes γ_j, similar to what was learned in the case of a strongly singular field only.

The same situation is studied in [N]. Spectral properties are of interest here, the means are quite different however. The vortices are treated as dynamical objects with their own kinetic energies. The special one-solenoid case is studied as well, and the splitting of a finite amount of eigenvalues from the Landau levels is predicted.

3.4 Generalized boundary conditions for the AB effect with a homogeneous magnetic field

This part is devoted to the study of the system described in 3.2.4. Thus, we consider a spinless charged quantum particle in two dimensions under the influence of a homogeneous magnetic field and the idealized AB effect.

This section contains the original results for this topic and is based on the article [EŠV].

3.4.1 Preliminaries

We consider the symmetric operator (cf. (3.7))

$$L = -(\nabla - A(\nabla))^2,\ D(L) = C_0^\infty(\mathbb{R}^2 \setminus \{0\}).$$

Then, all the definitions and assumptions from 3.2.4 hold true. Hence the potential A is given as $A = A_{\mathrm{hmf}} + A_{\mathrm{AB}}$, with

$$\begin{aligned} A_{\mathrm{hmf}} &= -\frac{\imath B}{2}(-x_2 dx_1 + x_1 dx_2), \\ A_{\mathrm{AB}} &= \frac{\imath \Phi}{2\pi r^2}(-x_2 dx_1 + x_1 dx_2), \\ r^2 &= x_1^2 + x_2^2. \end{aligned}$$

Then equally as before, $B > 0$, $\alpha = -\phi/2\pi$, and we assume that $\alpha \in (0, 1)$. Our goal is to describe all the self-adjoint extensions of L as well as to investigate their basic properties.

It is straightforward to determine the adjoint operator L^*,

$$\begin{aligned} \psi \in D(L^*) \quad \Longleftrightarrow \quad & \psi \in L^2(\mathbb{R}^2, \mathrm{d}^2x) \cap H^{2,2}_{\mathrm{loc}}(\mathbb{R}^2 \setminus \{0\}) \\ & \text{and } (\nabla - A(\nabla))^2 \psi \in L^2(\mathbb{R}^2, \mathrm{d}^2x). \end{aligned}$$

Next we can employ the rotational symmetry when using the polar coordinates (r, θ) and decomposing the Hilbert space into the orthogonal sum of the eigenspaces of the angular momentum,

$$L^2(\mathbb{R}^2, \mathrm{d}^2x) = \sum_{m \in \mathbb{Z}}^{\oplus} L^2(\mathbb{R}_+, r\,\mathrm{d}r) \otimes \mathbb{C}\, e^{\imath m \theta}. \tag{3.16}$$

In the polar coordinates the operator L (and correspondingly L^*) takes the form

$$L = -\frac{1}{r}\,\partial_r r \partial_r + \frac{1}{r^2}\left(-\imath\partial_\theta + \alpha + \frac{Br^2}{2}\right)^2.$$

The operator L^* commutes on $D(L^*)$ with the projectors P_m onto the eigenspaces of the angular momentum,

$$P_m\psi(r,\theta) = \frac{1}{2\pi}\int_0^{2\pi} \psi(r,\theta')\, e^{\imath m(\theta-\theta')}\, \mathrm{d}\theta',$$

and therefore L^* decomposes in correspondence with the orthogonal sum (3.16),

$$L^* = \sum_{m\in\mathbb{Z}}^{\oplus} (L^*)_m. \tag{3.17}$$

Thus we can reduce the problem and work in the sectors $\operatorname{Ran} P_m$, $m \in \mathbb{Z}$. For a given spectral parameter $\lambda \in \mathbb{C}$ we choose two independent solutions (except for some particular values of λ) of the differential equation

$$\left(-\frac{1}{r}\,\partial_r r \partial_r + \frac{1}{r^2}\left(m+\alpha+\frac{Br^2}{2}\right)^2\right) g(r) = \lambda\, g(r), \tag{3.18}$$

namely

$$\begin{aligned} g^1_m(\lambda;r) &= r^{|m+\alpha|}\, F\left(\beta(m,\lambda),\gamma(m),\frac{Br^2}{2}\right)\exp\left(-\frac{Br^2}{4}\right), \\ g^2_m(\lambda;r) &= r^{|m+\alpha|}\, G\left(\beta(m,\lambda),\gamma(m),\frac{Br^2}{2}\right)\exp\left(-\frac{Br^2}{4}\right), \end{aligned} \tag{3.19}$$

where

$$\begin{aligned} \beta(m,\lambda) &= \frac{1}{2}\left(1+m+\alpha+|m+\alpha|-\frac{\lambda}{B}\right), \\ \gamma(m) &= 1+|m+\alpha|\,. \end{aligned} \tag{3.20}$$

Here F and G are confluent hypergeometric functions [AS, Chp. 13],

$$F(\beta,\gamma,z) = \sum_{n=0}^{\infty} \frac{(\beta)_n\, z^n}{(\gamma)_n\, n!}\,,$$

and

$$G(\beta,\gamma,z) = \frac{\Gamma(1-\gamma)}{\Gamma(\beta-\gamma+1)}\, F(\beta,\gamma,z) + \frac{\Gamma(\gamma-1)}{\Gamma(\beta)}\, z^{1-\gamma} F(\beta-\gamma+1, 2-\gamma, z). \tag{3.21}$$

Notice that $F(\beta,\gamma,z)$ and $G(\beta,\gamma,z)$ are linearly dependent if and only if $\beta \in -\mathbb{Z}_+$. Moreover, $F(\beta,\gamma,z)$ is an entire function, particularly, it is

regular at the origin while $G(\beta,\gamma,z)$ has a singularity there provided $\gamma > 1$ and $\beta \notin -\mathbb{Z}_+$, and in that case it holds true that

$$\lim_{z\to 0_+} z^{\gamma-1} G(\beta,\gamma,z) = \frac{\Gamma(\gamma-1)}{\Gamma(\beta)}\,.$$

Thus in the case when $1 < \gamma < 2$ we have asymptotic behavior, as $z \to 0_+$,

$$G(\beta,\gamma,z) = \frac{\Gamma(\gamma-1)}{\Gamma(\beta)}\, z^{1-\gamma} + \frac{\Gamma(1-\gamma)}{\Gamma(\beta-\gamma+1)} + O(z^{2-\gamma}). \tag{3.22}$$

We shall also need some information about the asymptotic behavior at infinity. When $z \to +\infty$ it holds true that

$$F(\beta,\gamma,z) = \frac{\Gamma(\gamma)}{\Gamma(\gamma-\beta)}\,(-z)^{-\beta}\left(1 + O\left(z^{-1}\right)\right) + \frac{\Gamma(\gamma)}{\Gamma(\beta)}\, e^z z^{\beta-\gamma}\left(1 + O\left(z^{-1}\right)\right) \tag{3.23}$$

and

$$G(\beta,\gamma,z) = z^{-\beta}\left(1 + O\left(z^{-1}\right)\right).$$

3.4.2 The standard Aharonov-Bohm Hamiltonian

With the above preliminaries it is straightforward to solve the spectral problem for the standard AB Hamiltonian as we mentioned in the introduction. This means to solve the eigenvalue problem

$$L^*\psi = \lambda\psi$$

with the boundary condition

$$\lim_{r\to 0_+} \psi(r,\theta) = 0. \tag{3.24}$$

By virtue of the decomposition (3.17) the problem is reduced to countable set of equations

$$(L^*)_m f = \lambda f,\ m \in \mathbb{Z},$$

and hence to the differential equations (3.18).

The solution $g^2_m(\lambda; r)$ of (3.18) is ruled out because it contradicts the condition (3.24) and the solution $g^1_m(\lambda; r)$ belongs to $L^2(\mathbb{R}_+, r\,\mathrm{d}r)$ if and only if $\beta(m,\lambda) = -n$, with $n \in \mathbb{Z}_+$. Since it holds

$$F(-n, 1+\sigma, z) = \frac{n!\,\Gamma(\sigma+1)}{\Gamma(n+\sigma+1)}\, L^\sigma_n(z),\ n \in \mathbb{Z}_+,$$

we get a countable set of eigenvalues,

$$\lambda_{m,n} = B\,(m+\alpha+|m+\alpha|+2n+1),\ m\in\mathbb{Z},\ n\in\mathbb{Z}_+,$$

with the corresponding eigenfunctions

$$f_{m,n}(r,\theta) = C_{m,n}\, r^{|m+\alpha|}\, L_n^{|m+\alpha|}\left(\frac{Br^2}{2}\right)\,\exp\left(-\frac{Br^2}{4}\right)\,e^{\imath m\theta}$$

where

$$C_{m,n} = \left(\frac{B}{2}\right)^{\frac{1}{2}(|m+\alpha|+1)}\left(\frac{n!}{\pi\,\Gamma(n+|m+\alpha|+1)}\right)^{1/2}$$

are the normalisation constants.

As it is well known, if we fix $m\in\mathbb{Z}$ then the functions $\{f_{m,n}(r,\theta)\}_{n=0}^{\infty}$ form an orthonormal basis in $L^2(\mathbb{R}_+, r\,\mathrm{d}r)\otimes\mathbb{C}\,e^{\imath m\theta}$ and so the complete set of eigenfunctions $\{f_{m,n}(r,\theta)\}_{m\in\mathbb{Z},\ n\in\mathbb{Z}_+}$ is an orthonormal basis in $L^2(\mathbb{R}_+, r\,\mathrm{d}r)\otimes L^2([\,0,2\pi\,],\mathrm{d}\theta)$. Since all the eigenvalues $\lambda_{m,n}$ are real we get this way a well defined self-adjoint operator which is an extension of L. We conventionally call it the standard AB Hamiltonian and denote it by H^{AB}. Thus the spectrum of H^{AB} is pure point and can be written as a union of two parts,

$$\sigma(H^{AB}) = \sigma_{pp}(H^{AB}) = \{B(2k+1);\ k\in\mathbb{Z}_+\}\cup\{B(2\alpha+2k+1);\ k\in\mathbb{Z}_+\}.$$

Notice that the eigenvalues belonging to the first part are nothing but the Landau levels. All the eigenvalues $B(2k+1)$ have infinite multiplicities while the multiplicity of the eigenvalue $B(2\alpha+2k+1)$ is finite and equals $k+1$.

A final short remark concerning the Hamiltonian H^{AB} is devoted to the Green function. Naturally, the Green function is expressible as an infinite series

$$G^{AB}(z;r_1,\theta_1,r_2,\theta_2) = \frac{1}{2\pi}\sum_{m=-\infty}^{\infty} G_m^{AB}(z;r_1,r_2)\,e^{\imath m(\theta_1-\theta_2)}$$

where

$$\begin{aligned} G_m^{AB}(z;r_1,r_2) \;&=\; 2\left(\frac{B}{2}\right)^{|m+\alpha|+1}(r_1r_2)^{|m+\alpha|}\exp\left(-\frac{1}{4}\,B({r_1}^2+{r_2}^2)\right)\\ &\quad\times\sum_{n=0}^{\infty}\frac{n!}{\Gamma(n+|m+\alpha|+1)}\\ &\quad\times\frac{L_n^{|m+\alpha|}(\frac{1}{2}B{r_1}^2)\,L_n^{|m+\alpha|}(\frac{1}{2}B{r_2}^2)}{B(m+\alpha+|m+\alpha|+2n+1)-z}\,. \end{aligned}$$

The radial parts can be rewritten with the aid of the standard construction of the Green function for ordinary differential operators of the second order,

$$\begin{aligned} G_m^{AB}(z;r_1,r_2) &= \left(\frac{B}{2}\right)^{|m+\alpha|+1} (r_1 r_2)^{|m+\alpha|} \exp\left(-\frac{1}{4}\,B({r_1}^2+{r_2}^2)\right) \\ &\quad \times \frac{\Gamma\big(-w(m,z)\big)}{\Gamma(|m+\alpha|+1)}\, F(-w(m,z),|m+\alpha|+1,r_<) \\ &\quad \times G(-w(m,z),|m+\alpha|+1,r_>) \end{aligned}$$

where

$$w(m,z) = \frac{z}{2B} - \frac{1}{2}(m+\alpha+|m+\alpha|+1)$$

and $r_< = \min(r_1,r_2)$, $r_> = \max(r_1,r_2)$. This amounts to the identity

$$\begin{aligned} &\sum_{n=0}^{\infty} \frac{n!}{\Gamma(n+\sigma+1)}\, \frac{L_n^\sigma(y_1)\, L_n^\sigma(y_2)}{n-w} \\ &\qquad = \frac{\Gamma(-w)}{\Gamma(\sigma+1)}\, F(-w,\sigma+1,y_<)\, G(-w,\sigma+1,y_>). \end{aligned}$$

We do not expect that a simpler form for the Green function could be derived since the Hamiltonian H^{AB} enjoys only possesses rotational symmetry.

3.4.3 Self-adjoint extensions of L

Recalling what has been summarised in Section 3.4.1 it is easy to determine the deficiency indices. The solution $g_m^1(\pm\imath;r)$ diverges exponentially at infinity (cf. (3.23)) while $g_m^2(\pm\imath;r)$ behaves well at infinity but has a singularity at the origin of the order $r^{-|m+\alpha|}$. Thus $g_m^2(\pm\imath;r) \in L^2(\mathbb{R}_+, r\,\mathrm{d}r)$ if and only if $m=-1$ or $m=0$. This means that the deficiency indices are $(2,2)$. For a basis in the deficiency subspaces $\mathcal{N}_{\pm\imath}$ we can choose

$$\{f_{m,\pm}(r,\theta) = \frac{1}{\sqrt{2\pi}}\, N_m\, g_m^2(\pm\imath;r)\, e^{\imath m\theta};\ m=-1,0\}.$$

Thus

$$\begin{aligned} f_{-1,\pm}(r,\theta) &= \frac{1}{\sqrt{2\pi}}\, N_{-1}\, r^{1-\alpha}\, G\left(\frac{1}{2} \mp \frac{\imath}{2B}, 2-\alpha, \frac{Br^2}{2}\right) \exp\left(-\frac{Br^2}{4}\right) e^{-\imath\theta}, \\ f_{0,\pm}(r,\theta) &= \frac{1}{\sqrt{2\pi}}\, N_0\, r^{\alpha}\, G\left(\frac{1}{2}+\alpha \mp \frac{\imath}{2B}, 1+\alpha, \frac{Br^2}{2}\right) \exp\left(-\frac{Br^2}{4}\right), \end{aligned}$$

where N_{-1} and N_0 are the normalisation constants making the basis orthonormal.

We shall need the explicit values of N_{-1} and N_0. Using the relation

$$W_{\upsilon,\tau}(z) = z^{\tau+\frac{1}{2}} e^{-z/2}\, G\left(\frac{1}{2} - \upsilon + \tau, 2\tau + 1, z\right)$$

where W is the Whittaker function we get

$$\begin{aligned} N_m^{-2} &= \int_0^\infty |g_m^2(\pm\imath; r)|^2\, r\mathrm{d}r \\ &= \frac{1}{2}\left(\frac{2}{B}\right)^{|m+\alpha|+1} \int_0^\infty x^{-1} W_{\varrho,\sigma}(x)\, W_{\bar{\varrho},\sigma}(x)\, \mathrm{d}x \end{aligned}$$

where

$$\varrho = \frac{1}{2}\left(-m - \alpha + \frac{\imath}{B}\right),\ \sigma = \frac{1}{2}\,|m+\alpha|.$$

Combining the identities [PBM, 2.19.24.6]

$$\begin{aligned} \int_0^\infty x^{-1} W_{\varrho,\sigma}(x)\, W_{\mu,\sigma}(x)\, \mathrm{d}x &= \frac{\pi}{\sin(2\pi\sigma)} \\ &\times \left(-\frac{1}{\Gamma\left(\frac{1}{2} - \sigma - \mu\right)\, \Gamma\left(\frac{3}{2} + \sigma - \varrho\right)}\, {}_2F_1\left(\frac{1}{2} + \sigma - \mu, 1; \frac{3}{2} + \sigma - \varrho; 1\right) \right. \\ &\left. + \frac{1}{\Gamma\left(\frac{1}{2} + \sigma - \mu\right)\, \Gamma\left(\frac{3}{2} - \sigma - \varrho\right)}\, {}_2F_1\left(\frac{1}{2} - \sigma - \mu, 1; \frac{3}{2} - \sigma - \varrho; 1\right) \right) \end{aligned}$$

and

$$\begin{aligned} &{}_2F_1(a, b; c; z) = \\ &\frac{\Gamma(c)\,\Gamma(c-a-b)}{\Gamma(c-a)\,\Gamma(c-b)}\, {}_2F_1(a, b; a+b-c+1; 1-z) \\ &+ \frac{\Gamma(c)\,\Gamma(a+b-c)}{\Gamma(a)\,\Gamma(b)}\, (1-z)^{c-a-b}\, {}_2F_1(c-a, c-b; c-a-b+1; 1-z) \end{aligned}$$

we arrive at the relation

$$\begin{aligned} \int_0^\infty x^{-1} W_{\varrho,\sigma}(x)\, W_{\mu,\sigma}(x)\, \mathrm{d}x &= \frac{\pi}{\sin(2\pi\sigma)(\mu - \varrho)} \\ &\times \left(-\frac{1}{\Gamma\left(\frac{1}{2} - \mu - \sigma\right)\, \Gamma\left(\frac{1}{2} - \varrho + \sigma\right)} + \frac{1}{\Gamma\left(\frac{1}{2} - \mu + \sigma\right)\, \Gamma\left(\frac{1}{2} - \varrho - \sigma\right)} \right). \end{aligned}$$

Finally we get

$$N_{-1} = \left(\frac{B}{2}\right)^{\frac{1}{2}(1-\alpha)} \sqrt{\frac{\sin(\pi\alpha)}{2\pi}} \left(\operatorname{Im} \frac{1}{\Gamma\left(-\frac{1}{2}+\alpha+\frac{\imath}{2B}\right)\Gamma\left(\frac{1}{2}-\frac{\imath}{2B}\right)} \right)^{-1/2},$$

$$N_0 = \left(\frac{B}{2}\right)^{\frac{1}{2}\alpha} \sqrt{\frac{\sin(\pi\alpha)}{2\pi}} \left(\operatorname{Im} \frac{1}{\Gamma\left(\frac{1}{2}+\frac{\imath}{2B}\right)\Gamma\left(\frac{1}{2}+\alpha-\frac{\imath}{2B}\right)} \right)^{-1/2}.$$

Let us have a look at the asymptotic behavior at the origin of the basis functions in the deficiency subspaces $\mathcal{N}_{\pm\imath}$. By (3.19) and (3.22) we have

$$\begin{aligned} g^2_{-1}(\pm\imath; r) &= a_{-1,\pm}\, r^{-1+\alpha} + b_{-1,\pm}\, r^{1-\alpha} + O(r^{1+\alpha}), \\ g^2_{0}(\pm\imath; r) &= a_{0,\pm}\, r^{-\alpha} + b_{0,\pm}\, r^{\alpha} + O(r^{2-\alpha}), \end{aligned} \tag{3.25}$$

where

$$a_{-1,\pm} = \frac{\Gamma(1-\alpha)}{\Gamma\left(\frac{1}{2}\mp\frac{\imath}{2B}\right)} \left(\frac{B}{2}\right)^{-1+\alpha}, \quad b_{-1,\pm} = \frac{\Gamma(-1+\alpha)}{\Gamma\left(-\frac{1}{2}+\alpha\mp\frac{\imath}{2B}\right)},$$

$$a_{0,\pm} = \frac{\Gamma(\alpha)}{\Gamma\left(\frac{1}{2}+\alpha\mp\frac{\imath}{2B}\right)} \left(\frac{B}{2}\right)^{-\alpha}, \quad b_{0,\pm} = \frac{\Gamma(-\alpha)}{\Gamma\left(\frac{1}{2}\mp\frac{\imath}{2B}\right)}.$$

The coefficients $a_{m,\pm}$, $b_{m,\pm}$ are related to the normalisation constants N_m, for it holds true that

$$\det M_{-1} = -\frac{\imath}{1-\alpha}\,(N_{-1})^{-2}, \;\; \det M_0 = -\frac{\imath}{\alpha}\,(N_0)^{-2}. \tag{3.26}$$

where

$$M_m = \begin{pmatrix} a_{m,+} & b_{m,+} \\ a_{m,-} & b_{m,-} \end{pmatrix}.$$

Particularly, we shall need the fact that the matrices M_{-1} and M_0 are regular.

Let us now describe the closure of the operator L. By virtue of the decomposition (3.17) we have

$$\bar{L} = \sum_{m\in\mathbb{Z}}^{\oplus} \bar{L}_m$$

where $\bar{L}_m = (L^*)^*_m$. As it is well known, $\psi \in D(L^*)$ belongs to $D(\bar{L})$ if and only if $\langle \psi, L^*\varphi\rangle = \langle L^*\psi, \varphi\rangle$ for all $\varphi \in \mathcal{N}_\imath + \mathcal{N}_{-\imath}$. Thus $(L^*)_m = \bar{L}_m$ for $m \neq \{-1, 0\}$, and if $m \in \{-1, 0\}$ then $\varphi(r)\, e^{\imath m\theta} \in D((L^*)_m)$ belongs to $D(\bar{L}_m)$ if and only if

$$\lim_{r\to 0_+} r\, W(\overline{\varphi(r)}, g^2_m(\pm\imath, r)) = 0$$

where $W(f,g) = (\partial_r f)g - f\,\partial_r g$ is the Wronskian. Using the asymptotic behavior (3.25) and the regularity of matrix M_m we arrive at two conditions

$$\begin{aligned}\lim_{r\to 0_+}(-|m+\alpha|\, r^{-|m+\alpha|}\varphi(r) - r^{-|m+\alpha|+1}\partial_r\varphi(r)) = 0,\\ \lim_{r\to 0_+}(|m+\alpha|\, r^{|m+\alpha|}\varphi(r) - r^{|m+\alpha|+1}\partial_r\varphi(r)) = 0,\end{aligned}$$

which can be rewritten in the equivalent form,

$$\lim_{r\to 0_+} r^{-2|m+\alpha|+1}\partial_r(r^{|m+\alpha|}\varphi(r)) = 0, \quad \lim_{r\to 0_+} r^{|m+\alpha|}\varphi(r) = 0.$$

But since

$$r^{-|m+\alpha|}|\varphi(r)| \leq \frac{1}{2|m+\alpha|}\sup_{x\in\,]0,r[}|x^{-2|m+\alpha|+1}\partial_x(x^{|m+\alpha|}\varphi(x))|$$

we finally get a sufficient and necessary condition for $\varphi(r)\,e^{\imath m\theta} \in D((L^*)_m)$ to belong to $D(\bar{L})$, namely

$$\begin{aligned}&\lim_{r\to 0_+} r^{-1+\alpha}\varphi(r) = 0 \text{ and } \lim_{r\to 0_+} r^{\alpha}\varphi'(r) = 0 \qquad \text{if } m = -1,\\ &\lim_{r\to 0_+} r^{-\alpha}\varphi(r) = 0 \text{ and } \lim_{r\to 0_+} r^{-\alpha+1}\varphi'(r) = 0 \qquad \text{if } m = 0.\end{aligned} \tag{3.27}$$

This shows that if $\psi \in D(L^*) = D(\bar{L}) + \mathcal{N}_\imath + \mathcal{N}_{-\imath}$ then

$$\begin{aligned}\psi(r,\theta) &= \left(\Phi_1^1(\psi)r^{-1+\alpha} + \Phi_2^1(\psi)r^{1-\alpha}\right)e^{-\imath\theta} + \Phi_1^2(\psi)r^{-\alpha} + \Phi_2^2(\psi)r^{\alpha}\\ &\quad + \text{a regular part.}\end{aligned}$$

Let us formally introduce the functionals Φ_j^k on $D(L^*)$,

$$\Phi_1^{-1}(\psi) = \lim_{r\to 0_+} r^{1-\alpha}\frac{1}{2\pi}\int_0^{2\pi}\psi(r,\theta)\,e^{\imath\theta}\mathrm{d}\theta, \tag{3.28}$$

$$\Phi_2^{-1}(\psi) = \lim_{r\to 0_+} r^{-1+\alpha}\left(\frac{1}{2\pi}\int_0^{2\pi}\psi(r,\theta)\,e^{\imath\theta}\mathrm{d}\theta - \Phi_1^1(\psi)\,r^{-1+\alpha}\right), \tag{3.29}$$

$$\Phi_1^0(\psi) = \lim_{r\to 0_+} r^{\alpha}\frac{1}{2\pi}\int_0^{2\pi}\psi(r,\theta)\mathrm{d}\theta, \tag{3.30}$$

$$\Phi_2^0(\psi) = \lim_{r\to 0_+} r^{-\alpha}\left(\frac{1}{2\pi}\int_0^{2\pi}\psi(r,\theta)\mathrm{d}\theta - \Phi_1^2(\psi)\,r^{-\alpha}\right). \tag{3.31}$$

Notice that the upper index refers to the sector of angular momentum while the lower index refers to the order of the singularity. If $\psi \in D(\bar{L})$ then according to (3.27) it actually holds $\Phi_j^k(\psi) = 0$ for $j = 1,2$, $k = -1,0$. On the other hand, if $\psi \in \mathcal{N}_\imath + \mathcal{N}_{-\imath}$ and $\Phi_j^k(\psi) = 0$ for all indices $j = 1,2$,

$k = -1, 0$, then $\psi = 0$ (this is again guaranteed by the regularity of the matrices M_{-1} and M_0).

Let us introduce some more notation. It is convenient to arrange the functionals Φ_j^k into column vectors as follows,

$$\Phi_j(\psi) = \begin{pmatrix} \Phi_j^{-1}(\psi) \\ \Phi_j^0(\psi) \end{pmatrix}, \ j = 1, 2.$$

Further, applying the functionals to the basis functions in $\mathcal{N}_\imath + \mathcal{N}_{-\imath}$, we obtain four 2×2 diagonal matrices. More precisely, set

$$(\Phi_{j,\pm})_{k\ell} = \sqrt{2\pi}\, \Phi_j^{k-2}(f_{\ell-2,\pm}), \ j, k, \ell = 1, 2.$$

Then

$$\Phi_{1,\pm} = \begin{pmatrix} N_{-1} a_{-1,\pm} & 0 \\ 0 & N_0\, a_{0,\pm} \end{pmatrix}, \ \Phi_{2,\pm} = \begin{pmatrix} N_{-1} b_{-1,\pm} & 0 \\ 0 & N_0\, b_{0,\pm} \end{pmatrix}.$$

Now it is straightforward to give a formal definition of a self-adjoint extension H^U of the symmetric operator L determined by a unitary operator $U : \mathcal{N}_\imath \to \mathcal{N}_{-\imath}$. We identify U with a unitary 2×2 matrix via the choice of the orthonormal bases $\{f_{-1,\pm}, f_{0,\pm}\}$ in $\mathcal{N}_{\pm\imath}$.The self-adjoint operator H^U is unambiguously defined by the condition: $H^U \subset L^*$ and $\psi \in D(L^*)$ belongs to $D(H^U)$ if and only if

$$\begin{pmatrix} \Phi_1(\psi) \\ \Phi_2(\psi) \end{pmatrix} \in \mathrm{Ran} \begin{pmatrix} \Phi_{1,+} + \Phi_{1,-} U \\ \Phi_{2,+} + \Phi_{2,-} U \end{pmatrix}. \tag{3.32}$$

However condition (3.32) is rather inconvenient and we shall replace it in the next section by another one more suitable for practical purposes.

3.4.4 Boundary conditions

To turn (3.32) into a convenient requirement which would involve boundary conditions we shall need the following proposition. Set

$$D = \begin{pmatrix} 1 - \alpha & 0 \\ 0 & \alpha \end{pmatrix}.$$

There is a one-to-one correspondence between the unitary matrices $U \in U(2)$ and the couples of matrices $X_1, X_2 \in \mathrm{Mat}(2, \mathbb{C})$ obeying

$$\mathrm{rank} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = 2 \tag{3.33}$$

and

$$X_1^* D X_2 = X_2^* D X_1 \tag{3.34}$$

modulo the right action of the group of regular matrices $GL(2,\mathbb{C})$*. The one-to-one correspondence is given by the equality*

$$\mathrm{Ran}\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \in \mathrm{Ran}\begin{pmatrix} \Phi_{1,+} + \Phi_{1,-}U \\ \Phi_{2,+} + \Phi_{2,-}U \end{pmatrix}.$$

Let us note that the equivalence class of the couple (X_1, X_2) modulo $GL(2,\mathbb{C})$ corresponds to a two-dimensional subspace in $\mathbb{C}^4$ and hence to a point in the Grassmann manifold $\mathbb{G}_2(\mathbb{C}^4)$. The complex dimension of $\mathbb{G}_2(\mathbb{C}^4)$ equals 4, i.e. $\dim_{\mathbb{R}} \mathbb{G}_2(\mathbb{C}^4) = 8$. The points of $\mathbb{G}_2(\mathbb{C}^4)$ obeying the ("real") condition (3.34) form a real 4-dimensional submanifold which is diffeomorphic, according to the proposition, to the unitary group $U(2)$.

To verify the proposition we first show that to any couple (X_1, X_2) with the properties (3.33), (3.34) there are related unique $Y \in GL(2,\mathbb{C})$ and $U \in U(2)$ such that

$$\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} Y = \boldsymbol{J} \begin{pmatrix} I \\ U \end{pmatrix} \tag{3.35}$$

where we have set

$$\boldsymbol{J} = \begin{pmatrix} \Phi_{1,+} & \Phi_{1,-} \\ \Phi_{2,+} & \Phi_{2,-} \end{pmatrix} = \begin{pmatrix} N_{-1}a_{-1,+} & 0 & N_{-1}a_{-1,-} & 0 \\ 0 & N_0 a_{0,+} & 0 & N_0 a_{0,-} \\ N_{-1}b_{-1,+} & 0 & N_{-1}b_{-1,-} & 0 \\ 0 & N_0 b_{0,+} & 0 & N_0 b_{0,-} \end{pmatrix}.$$

Using (3.26) one easily finds that $\boldsymbol{J}$ is regular and

$$\boldsymbol{J}^{-1} = \imath \begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix} \begin{pmatrix} \Phi_{2,-} & -\Phi_{1,-} \\ -\Phi_{2,+} & \Phi_{1,+} \end{pmatrix}.$$

Let us introduce another couple of matrices, $V_+, V_- \in \mathrm{Mat}(2,\mathbb{C})$, by the relation

$$\begin{pmatrix} V_- \\ V_+ \end{pmatrix} = \boldsymbol{J}^{-1} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix},$$

thus $V_\pm = \mp \imath D(\Phi_{2,\pm} X_1 - \Phi_{1,\pm} X_2)$. It follows that

$$V_\pm^* V_\pm = \begin{pmatrix} X_1^* & X_2^* \end{pmatrix} \begin{pmatrix} \Phi_{2,\pm}^* D^2 \Phi_{2,\pm} & -\Phi_{2,\pm}^* D^2 \Phi_{1,\pm} \\ -\Phi_{1,\pm}^* D^2 \Phi_{2,\pm} & \Phi_{1,\pm}^* D^2 \Phi_{1,\pm} \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}$$

and, consequently,

$$V_-^* V_- - V_+^* V_+ = \begin{pmatrix} X_1^* & X_2^* \end{pmatrix} \begin{pmatrix} 0 & -\imath D \\ \imath D & 0 \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \imath (X_2^* D X_1 - X_1^* D X_2)$$

for $\Phi_{j,\pm}$ and D commute (all of them are diagonal), $\Phi_{j,\pm}^* = \Phi_{j,\mp}$ and

$$-\Phi_{1,+}\Phi_{2,-} + \Phi_{1,-}\Phi_{2,+} = \imath D^{-1}$$

(cf. (3.26)). Owing to the property (3.34) we have

$$V_-^* V_- = V_+^* V_+ \tag{3.36}$$

which jointly with property (3.33) implies that

$$\operatorname{Ker} V_- = \operatorname{Ker} V_+ = \operatorname{Ker} \begin{pmatrix} V_- \\ V_+ \end{pmatrix} = \operatorname{Ker} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = 0.$$

The only possible choice of the matrices Y and U satisfying (3.35) is

$$Y = V_-^{-1},\ U = V_+ V_-^{-1}.$$

The matrix U is actually unitary because of (3.36).

Conversely, we have to show that any couple of matrices X_1, X_2 related to a unitary matrix U according to the rule

$$\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \boldsymbol{J} \begin{pmatrix} I \\ U \end{pmatrix}$$

obeys (3.33) and (3.34). Condition (3.33) is obvious since $\boldsymbol{J}$ is regular and condition (3.34) is again a matter of a direct computation. In more detail, since it holds

$$X_1^* D X_2 - X_2^* D X_1 = \begin{pmatrix} I & U^* \end{pmatrix} \boldsymbol{J}^* \begin{pmatrix} 0 & D \\ -D & 0 \end{pmatrix} \boldsymbol{J} \begin{pmatrix} I \\ U \end{pmatrix}$$

it suffices to verify that

$$\boldsymbol{J}^* \begin{pmatrix} 0 & D \\ -D & 0 \end{pmatrix} \boldsymbol{J} = \imath \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}.$$

This concludes the proof of the above proposition.

Using this correspondence one can relate to a couple $X_1, X_2 \in \operatorname{Mat}(2, \mathbb{C})$ obeying (3.33) and (3.34) a self-adjoint extension H determined by the condition

$$\psi \in D(H) \Longleftrightarrow \begin{pmatrix} \Phi_1(\psi) \\ \Phi_2(\psi) \end{pmatrix} \in \operatorname{Ran} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}. \tag{3.37}$$

Two couples (X_1, X_2) and (X_1', X_2') determine the same self-adjoint extension if and only if there exists a regular matrix Y such that $(X_1', X_2') =$

(X_1Y, X_2Y). Moreover, all the self-adjoint extensions can be obtained in this way.

We shall restrict ourselves to an open dense subset in the space of all self-adjoint extensions by requiring the matrix X_2 to be regular. In that case we can set directly $X_2 = I$ and rename $X_1 = \Lambda$. Thus Λ is a 2×2 complex matrix satisfying

$$D\Lambda = \Lambda^* D. \tag{3.38}$$

The corresponding self-adjoint extension will be denoted H^Λ. The condition (3.37) simplifies in an obvious way. We conclude that $H^\Lambda \subset L^*$ and $\psi \in D(L^*)$ belongs to $D(H^\Lambda)$ if and only if

$$\Phi_1(\psi) = \Lambda \Phi_2(\psi), \tag{3.39}$$

and this is in fact the sought boundary condition.

Matrices Λ obeying (3.38) can be parametrised by four real parameters (or two real and one complex). We choose the parameterisation

$$\Lambda = \begin{pmatrix} u & \alpha\bar{w} \\ (1-\alpha)w & v \end{pmatrix}, \ u, v \in \mathbb{R}, \ w \in \mathbb{C}.$$

The relation between Λ and U reads

$$\Lambda = (\Phi_{1,+} + \Phi_{1,-}U)(\Phi_{2,+} + \Phi_{2,-}U)^{-1} \tag{3.40}$$

(provided the RHS makes sense).

The "most regular" among the boundary conditions is $\Phi_1(\psi) = 0$, i.e. the one determined by $\Lambda = 0$, and the corresponding self-adjoint extension is nothing but the standard Aharonov-Bohm Hamiltonian H^{AB} discussed in Section 3.4.2. According to (3.40) H^{AB} corresponds to the unitary matrix

$$U = -\Phi_{1,-}^{-1}\Phi_{1,+} = \operatorname{diag}\left\{ -\frac{\Gamma\left(\frac{1}{2} + \frac{\imath}{2B}\right)}{\Gamma\left(\frac{1}{2} - \frac{\imath}{2B}\right)}, -\frac{\Gamma\left(\frac{1}{2} + \alpha + \frac{\imath}{2B}\right)}{\Gamma\left(\frac{1}{2} + \alpha - \frac{\imath}{2B}\right)} \right\}.$$

3.4.5 The spectrum

Let us now proceed to the discussion of spectral properties of the described self-adjoint extensions. It is clear from what has been explained up to now that everything interesting is happening in the two critical sectors of the angular momentum labeled by $m = -1$ and $m = 0$. To state it more formally we decompose the Hilbert space into an orthogonal sum of the "stable" and "critical" parts,

$$\mathcal{H} = \mathcal{H}_s \oplus \mathcal{H}_c$$

where

$$\mathcal{H}_s = \sum_{m\in\mathbb{Z}\setminus\{-1,0\}}^{\oplus} L^2(\mathbb{R}_+, r\,\mathrm{d}r)\otimes \mathbb{C}\, e^{\imath m\theta},\ \mathcal{H}_c = L^2(\mathbb{R}_+, r\,\mathrm{d}r)\otimes(\mathbb{C}\, e^{-\imath\theta}\oplus \mathbb{C}\,1).$$

A self-adjoint extension H^Λ decomposes correspondingly,

$$H^\Lambda = H^\Lambda|_{\mathcal{H}_s} \oplus H^\Lambda|_{\mathcal{H}_c}\,,$$

and we know that on $\mathcal{H}_s$ the operator H^Λ coincides with the standard AB Hamiltonian,

$$H^\Lambda|_{\mathcal{H}_s} = H^{AB}|_{\mathcal{H}_s}.$$

Thus

$$\sigma(H^\Lambda) = \sigma(H^{AB}|_{\mathcal{H}_s}) \cup \sigma(H^\Lambda|_{\mathcal{H}_c})$$

and, as explained in Section 3.4.2,

$$\sigma(H^{AB}|_{\mathcal{H}_s}) = \{B(2k+1);\ k\in\mathbb{Z}_+\}\cup\{B(2k+2\alpha+1);\ k\in\mathbb{N}\}$$

where the multiplicity of the eigenvalue $B(2k+1)$ is infinite while the multiplicity of the eigenvalue $B(2k+2\alpha+1)$ equals k. On the other hand,

$$\sigma(H^{AB}|_{\mathcal{H}_c}) = \{B(2k+1);\ k\in\mathbb{Z}_+\}\cup\{B(2k+2\alpha+1);\ k\in\mathbb{Z}_+\}$$

where all the eigenvalues are simple (the first set is the contribution of the sector $m=-1$ while the second one comes from the sector $m=0$). Since the deficiency indices are finite, the Krein's formula jointly with Weyl Theorem [RS2, Theorem XIII.14] tells us that the essential spectrum $\sigma_{ess}(H^\Lambda|_{\mathcal{H}_c})$ is empty for any Λ. Thus the spectrum of $H^\Lambda|_{\mathcal{H}_c}$ is formed by eigenvalues which are at most finitely degenerated and have no finite accumulation points.

Let us derive the equation on eigenvalues for the restriction $H^\Lambda|_{\mathcal{H}_c}$. Let $\lambda\in\mathbb{R}$. In each of the sectors $m=-1,0$ there exists exactly one (up to a multiplicative constant) solution of the equation $(L^*)_m f = \lambda f$ which is L^2-integrable at infinity (with respect to the measure $r\,\mathrm{d}r$) and we may take for it the function $g^2_m(\lambda;r)\,e^{\imath m\theta}$ (cf. (3.19)). For a second linearly independent solution one may take $g^1_m(\lambda;r)\,e^{\imath m\theta}$ provided $\beta(m,\lambda)\notin -\mathbb{Z}_+$ (cf. (3.20)). If $\beta(m,\lambda)\in-\mathbb{Z}_+$ then a possible choice of the second linearly independent solution is

$$r^{|m+\alpha|}\,H\left(\beta(m,\lambda),\gamma(m),\frac{Br^2}{2}\right)\,\exp\left(-\frac{Br^2}{4}\right)$$

where

$$H(\beta,\gamma,z) = z^{1-\gamma}F(\beta-\gamma+1,2-\gamma,z)$$

(cf. (3.21)).

Thus λ is an eigenvalue of $H^\Lambda|_{\mathcal{H}_c}$ if and only if there exists a vector $(\mu,\nu)\in\mathbb{C}^2\setminus\{0\}$ such that the function

$$\psi_\lambda(r,\theta)=\mu\, g^2_{-1}(\lambda;r)\, e^{-\imath\theta}+\nu\, g^2_0(\lambda;r)$$

satisfies the boundary condition (3.39). Using again (3.19) and (3.22) one finds that

$$\Phi_1(\psi_\lambda)=\begin{pmatrix} a_{-1} & 0\\ 0 & a_0\end{pmatrix}\begin{pmatrix}\mu\\ \nu\end{pmatrix},\ \Phi_2(\psi_\lambda)=\begin{pmatrix} b_{-1} & 0\\ 0 & b_0\end{pmatrix}\begin{pmatrix}\mu\\ \nu\end{pmatrix},$$

where

$$\begin{aligned} a_{-1}&=\frac{\Gamma(1-\alpha)}{\Gamma\left(\frac12-\frac{\lambda}{2B}\right)}\left(\frac{B}{2}\right)^{-1+\alpha}\quad,\quad b_{-1}=\frac{\Gamma(-1+\alpha)}{\Gamma\left(-\frac12+\alpha-\frac{\lambda}{2B}\right)},\\ a_0&=\frac{\Gamma(\alpha)}{\Gamma\left(\frac12+\alpha-\frac{\lambda}{2B}\right)}\left(\frac{B}{2}\right)^{-\alpha}\quad,\quad b_0=\frac{\Gamma(-\alpha)}{\Gamma\left(\frac12-\frac{\lambda}{2B}\right)}.\end{aligned}$$

This immediately leads to the desired equation on eigenvalues which takes the form $\det \boldsymbol{A}=0$ where

$$\boldsymbol{A}=\begin{pmatrix} a_{-1} & 0\\ 0 & a_0\end{pmatrix}\begin{pmatrix}\mu\\ \nu\end{pmatrix}-\Lambda\begin{pmatrix} b_{-1} & 0\\ 0 & b_0\end{pmatrix}.$$

After the substitution

$$z=\frac12-\frac{\lambda}{2B},\ \text{i.}e.\ \lambda=B(1-2z),$$

we get

$$\begin{aligned}&\frac{\Gamma(1-\alpha)\Gamma(\alpha)}{\Gamma(z)\Gamma(z+\alpha)}\,\frac{2}{B}-\frac{\Gamma(\alpha)\Gamma(\alpha-1)}{\Gamma(z+\alpha-1)\Gamma(z+\alpha)}\left(\frac{2}{B}\right)^{\alpha}u\\ &\quad-\frac{\Gamma(1-\alpha)\Gamma(-\alpha)}{\Gamma(z)^2}\left(\frac{2}{B}\right)^{1-\alpha}v\\ &\quad+\frac{\Gamma(\alpha-1)\Gamma(-\alpha)}{\Gamma(z)\Gamma(z+\alpha-1)}\left(uv-\alpha(1-\alpha)|w|^2\right)\,=\,0.\end{aligned}$$

To simplify somewhat the form of the equation it is convenient to rescale the parameters as follows,

$$\xi=\left(\frac{B}{2}\right)^{1-\alpha}\frac{\Gamma(\alpha)}{\Gamma(2-\alpha)}\,u,\ \eta=\left(\frac{B}{2}\right)^{\alpha}\frac{\Gamma(1-\alpha)}{\Gamma(1+\alpha)}\,v,\ \zeta=\sqrt{\frac{B}{2}}\,|w|.\qquad(3.41)$$

Finally we arrive at an equation depending on three real parameters ξ, η, ζ, namely

$$\frac{1}{\Gamma(z)\,\Gamma(z+\alpha)} + \frac{\xi}{\Gamma(z+\alpha-1)\,\Gamma(z+\alpha)} + \frac{\eta}{\Gamma(z)^2} + \frac{\xi\,\eta - \zeta^2}{\Gamma(z)\,\Gamma(z+\alpha-1)} = 0. \tag{3.42}$$

There is no chance to solve equation (3.42) explicitly apart of some particular cases. One of them, of course, corresponds to the standard AB Hamiltonian. This case is determined by the values of parameters $\xi = \eta = \zeta = 0$ and the roots of (3.42) form the set $-\mathbb{Z}_+ \cup (-\alpha - \mathbb{Z}_+)$. Consider also the case when $\xi = \eta = 0$ and $\zeta \neq 0$ with the set of roots equal to $-\mathbb{Z}_+ \cup (-\alpha - \mathbb{Z}_+) \cup \{1 - \alpha + \zeta^{-2}\}$. Comparing the latter case to the former one we see that there is one additional root, namely $1 - \alpha + \zeta^{-2}$, which escapes to infinity when $\zeta \to 0$.

In the last particular case one can also consider the limit $\zeta \to \infty$. More generally, suppose that $\det \Lambda \neq 0$, i.e. $\xi\eta - \zeta^2 \neq 0$, replace Λ with $t\,\Lambda$ in (3.39) and take the limit $t \to \infty$. The limiting boundary condition reads

$$\Phi_2(\psi) = 0$$

and the corresponding self-adjoint extension which we shall call H^∞ is one of those omitted when we restricted ourselves to an open dense subset in the space of all self-adjoint extensions (regarded as a a 4-dimensional real manifold). Equation (3.42) reduces in this limit to the equation

$$\frac{1}{\Gamma(z)\,\Gamma(z+\alpha-1)} = 0 \tag{3.43}$$

with the set of roots $-\mathbb{Z}_+ \cup (1 - \alpha - \mathbb{Z}_+)$.

Another case when equation (3.42) simplifies yet it is not solvable explicitly is $\zeta = 0$. This is easy to understand since if $\zeta = 0$ then the matrix Λ is diagonal and the two critical sectors of angular momentum do not interfere. This is reflected in the fact that the equation (3.42) decomposes into two independent equations,

$$\frac{1}{\Gamma(z)} + \frac{\xi}{\Gamma(z+\alpha-1)} = 0, \;\; \frac{1}{\Gamma(z+\alpha)} + \frac{\eta}{\Gamma(z)} = 0.$$

Let us shortly discuss the dependence of the roots of equation (3.42) on parameters ξ, η, ζ. Since the derivative of the LHS of (3.42) with respect to z and with the values of parameters $(\xi, \eta, \zeta) = (0, 0, 0)$ equals

$$\frac{(-1)^m m!}{\Gamma(-m+\alpha)} \neq 0 \text{ for } z = -m, \text{ and } \frac{(-1)^m m!}{\Gamma(-m-\alpha)} \neq 0 \text{ for } z = -m - \alpha,$$

where $m \in \mathbb{Z}_+$, the standard Implicit Function Theorem (analytic case) is sufficient to conclude that the roots are analytic functions in ξ, η, ζ at least in some neighbourhood of the origin (depending in general on the root). Let us denote by $z_{1,m}(\xi,\eta,\zeta)$ and $z_{2,m}(\xi,\eta,\zeta)$ the roots of (3.42) regarded as analytic functions in ξ, η, ζ and such that $z_{1,m}(0,0,0) = -m$ and $z_{2,m}(0,0,0) = -\alpha - m$, with $m \in \mathbb{Z}_+$. A straightforward computation results in the following power series truncated at degree 4.

Set

$$\begin{aligned} h^0_m(z) &= \sum_{j=1}^{m} \frac{1}{j} - \gamma - \psi(z), \\ h^1_m(z) &= \frac{\pi^2}{6} + \sum_{j=1}^{m} \frac{1}{j^2} - \psi'(z), \\ h^2_m(z) &= -2\,\boldsymbol{\zeta}(3) + 2\sum_{j=1}^{m} \frac{1}{j^3} - \psi''(z), \end{aligned}$$

where γ is the Euler constant, $\psi(z) = \Gamma'(z)/\Gamma(z)$ is the digamma function and $\boldsymbol{\zeta}$ is the zeta function. Then

$$\begin{aligned} z_{1,m}(\xi,\eta,\zeta) &= -m + \frac{(-1)^{m+1}}{m!\,\Gamma(-1-m+\alpha)}\,\xi + \frac{h^0_m(-1-m+\alpha)}{(m!)^2\,\Gamma(-1-m+\alpha)^2}\,\xi^2 \\ &\quad + \frac{(-1)^{m+1}\left(3\,h^0_m(-1-m+\alpha)^2 + h^1_m(-1-m+\alpha)\right)}{2\,(m!)^3\,\Gamma\left(-1-m+\alpha\right)^3}\,\xi^3 \\ &\quad + \frac{(-1)^m\ (1+m-\alpha)}{m!\,\Gamma(-1-m+\alpha)}\,\xi\,\zeta^2 \\ &\quad + \frac{1}{6\,(m!)^4\,\Gamma(-1-m+\alpha)^4}\left(4\,h^0_m(-1-m+\alpha)\right. \\ &\quad \times \left(4\,h^0_m(-1-m+\alpha)^2 + 3\,h^2_m(-1-m+\alpha)\right) \\ &\quad \left. + h^2_m(-1-m+\alpha)\right)\xi^4 \\ &\quad + \frac{3 - 2\,(1+m-\alpha)\,h^0_m(-m+\alpha)}{(m!)^2\,\Gamma(-1-m+\alpha)^2}\,\xi^2\zeta^2 + \cdots, \end{aligned} \tag{3.44}$$

$$
\begin{aligned}
z_{2,m}(\xi,\eta,\zeta) \;=\;& -\alpha - m + \frac{(-1)^{m+1}}{m!\,\Gamma(-m-\alpha)}\,\eta + \frac{h^0_m(-m-\alpha)}{(m!)^2\,\Gamma(-m-\alpha)^2}\,\eta^2 \\
&+ \frac{(-1)^{m+1}\,(3\,h^0_m(-m-\alpha)^2 + h^1_m(-m-\alpha))}{2\,(m!)^3\,\Gamma\,(-m-\alpha)^3}\,\eta^3 \\
&+ \frac{(-1)^m\,(m+1)}{m!\,\Gamma(-m-\alpha)}\,\eta\,\zeta^2 \\
&+ \frac{1}{6\,(m!)^4\,\Gamma(-m-\alpha)^4}\,\big(4\,h^0_m(-m-\alpha) \\
&\quad \times \big(4\,h^0_m(-m-\alpha)^2 + 3\,h^2_m(-m-\alpha)\big) \\
&\quad + h^2_m(-m-\alpha)\big)\,\eta^4 \\
&+ \frac{1 - 2\,(m+1)\,h^0_m(-m-\alpha)}{(m!)^2\,\Gamma(-m-\alpha)^2}\,\eta^2\zeta^2 + \cdots\,.
\end{aligned}
\tag{3.45}
$$

A similar analysis can be carried out to get the asymptotic behavior of the roots for ξ, η, ζ large. To this end assume that $\xi\eta - \zeta^2 \neq 0$ and set

$$
\xi' = \frac{\xi}{\xi\eta - \zeta^2}\,,\;\; \eta' = \frac{\eta}{\xi\eta - \zeta^2}\,,\;\; \zeta' = \frac{\zeta}{\xi\eta - \zeta^2}\,.
$$

Notice that $\xi'\eta' - \zeta'^2 = (\xi\eta - \zeta^2)^{-1}$. Equation (3.42) becomes

$$
\frac{\xi'\eta' - \zeta'^2}{\Gamma(z)\,\Gamma(z+\alpha)} + \frac{\xi'}{\Gamma(z+\alpha-1)\,\Gamma(z+\alpha)} + \frac{\eta'}{\Gamma(z)^2} + \frac{1}{\Gamma(z)\,\Gamma(z+\alpha-1)} = 0. \tag{3.46}
$$

Roots of (3.46) are analytic functions in ξ', η', ζ' at least in some neighbourhood of the origin. Again, it would be possible to compute the beginning of the corresponding power series and to derive formulae similar to those of (3.44), (3.45) but we avoid doing it here explicitly.

Instead we prefer to plot two graphs in order to give the reader some impression about how the eigenvalues may depend on the parameters, i.e. on the boundary conditions. In each graph we choose a line in the parameter space, $\{(\xi t, \eta t, \zeta t) \in \mathbb{R}^3;\; t \in \mathbb{R}\}$, and we depict the dependence on t of several first eigenvalues for the corresponding self-adjoint extension restricted to $\mathcal{H}_c$ (see (3.41) for the substitution). In both graphs we have set $\alpha = 0.3$ and $B = 1$.

Probably the most complete general information which is available about solutions of equation (3.42) might be the localisation of roots of this equation with respect to a suitable splitting of the real line into intervals. Let us choose the splitting into intervals with boundary points coinciding with the roots of equation (3.43). To get the localisation let us rewrite equation (3.42), equivalently provided $z \neq -\mathbb{Z}_+ \cup (1 - \alpha - \mathbb{Z}_+)$, as follows

interval $(1-\alpha, +\infty)$			
conditions			number of roots
$\xi \geq 0$	$\eta \geq 0$	$\zeta^2 > \xi\eta$	1
$\xi \geq 0$	$\eta \geq 0$	$\zeta^2 \leq \xi\eta$	0
$\xi \geq 0$	$-\Gamma(1-\alpha) < \eta < 0$	no condition	1
$\xi \geq 0$	$\eta \leq -\Gamma(1-\alpha)$	no condition	0
$\xi < 0$	$\eta \geq 0$	no condition	1
$\xi < 0$	$-\Gamma(1-\alpha) < \eta < 0$	$\zeta^2 \geq \xi\eta$	1
$\xi < 0$	$-\Gamma(1-\alpha) < \eta < 0$	$\zeta^2 < \xi\eta$	2
$\xi < 0$	$\eta \leq -\Gamma(1-\alpha)$	$\zeta^2 \geq \xi\eta$	0
$\xi < 0$	$\eta \leq -\Gamma(1-\alpha)$	$\zeta^2 < \xi\eta$	1

Figure 3.5: Number of roots in interval $(1-\alpha, +\infty)$

interval $(0, 1-\alpha)$		
conditions		number of roots
$\xi \leq 0$	$\eta \geq -\Gamma(1-\alpha)$	0
$\xi \leq 0$	$\eta < -\Gamma(1-\alpha)$	1
$\xi > 0$	$\eta \geq -\Gamma(1-\alpha)$	1
$\xi > 0$	$\eta < -\Gamma(1-\alpha)$	2

Figure 3.6: Number of roots in interval $(0, 1-\alpha)$

$$\left(\frac{\Gamma(z-1+\alpha)}{\Gamma(z)} + \xi\right)\left(\frac{\Gamma(z)}{\Gamma(z+\alpha)} + \eta\right) = \zeta^2. \tag{3.47}$$

Put

$$F_\alpha(z) = \frac{\Gamma(z-1+\alpha)}{\Gamma(z)}$$

so that equation (3.47) can be rewritten as

$$\left(F_\alpha(z) + \xi\right)\left(F_{1-\alpha}(z+\alpha) + \eta\right) = \zeta^2. \tag{3.48}$$

It is easy to carry out some basic analysis of the function $F_\alpha(z)$. We have ${F_\alpha}'(z) = F_\alpha(z)\left(\psi(z-1+\alpha) - \psi(z)\right)$. One observes that $F_\alpha(z) > 0$ for $z \in \,]1-\alpha, +\infty[\, \cup \left(\bigcup_{m\in\mathbb{Z}_+} \,]-\alpha-m, -m[\,\right)$, and $F_\alpha(z) < 0$ for $z \in \bigcup_{m\in\mathbb{Z}_+} \,]-m, 1-\alpha-m[\,$, and in any case ${F_\alpha}'(z) < 0$. In the former case this follows from the fact that $\psi(z)$ is strictly increasing on each of the intervals $\,]0, +\infty[\,$ and $\,]-m-1, -m[\,$, with $m \in \mathbb{Z}_+$. In the latter case this

intervals $(-\alpha-m,-m), m\in\mathbb{Z}_+$		
conditions		number of roots
$\xi\geq 0$	$\eta\leq 0$	0
$\xi\geq 0$	$\eta>0$	1
$\xi<0$	$\eta\leq 0$	1
$\xi<0$	$\eta>0$	2

Figure 3.7: Number of roots in intervals $(-\alpha-m,-m), m\in\mathbb{Z}_+$

intervals $(-1-m,-\alpha-m), m\in\mathbb{Z}_+$		
conditions		number of roots
$\xi\leq 0$	$\eta\geq 0$	0
$\xi\leq 0$	$\eta<0$	1
$\xi>0$	$\eta\geq 0$	1
$\xi>0$	$\eta<0$	2

Figure 3.8: Number of roots in intervals $(-1-m,-\alpha-m), m\in\mathbb{Z}_+$

is a consequence of the identity

$$\psi(z-1+\alpha)-\psi(z)=\frac{\pi\,\sin(\pi\alpha)}{\sin(\pi z)\,\sin(\pi(z+\alpha))}+\int_0^\infty \frac{e^{-(1-z)\,t}\left(1-e^{-(1-\alpha)\,t}\right)}{1-e^{-t}}\,\mathrm{d}t.$$

Moreover,

$$\lim_{z\to+\infty}F_\alpha(z)=0,\quad \lim_{z\to(1-\alpha-m)\pm}F_\alpha(z)=\pm\infty \text{ and } F_\alpha(-m)=0 \text{ for } m\in\mathbb{Z}_+.$$

This also implies that $F_{1-\alpha}(z+\alpha)>0$ for every z such that $z\in\,]0,+\infty[\,\cup\left(\bigcup_{m\in\mathbb{Z}_+}\,]-1-m,-\alpha-m[\right)$ and $F_{1-\alpha}(z)<0$ for $z\in\bigcup_{m\in\mathbb{Z}_+}\,]-\alpha-m,-m[$, in any case ${F_{1-\alpha}}'(z+\alpha)<0$, and

$$\lim_{z\to+\infty}F_{1-\alpha}(z+\alpha)=0,\quad \lim_{z\to-m\pm}F_{1-\alpha}(z+\alpha)=\pm\infty,$$
$$\text{and } F_{1-\alpha}(-\alpha-m)=0 \text{ for } m\in\mathbb{Z}_+.$$

With the knowledge of these basic properties of the function $F_\alpha(z)$ it is a matter of an elementary analysis to determine the number of roots of equation (3.48) in each of the intervals $]1-\alpha,+\infty[\,,\ ]-m,1-\alpha-m[$ and $]-\alpha-m,-m[\,$, with $m\in\mathbb{Z}_+$. The result is summarized in the following tables.

This is to be completed with the simple observation that $1-\alpha$ is a root of (3.42) if and only if $\eta=-\Gamma(1-\alpha)$, and $-m$, with $m\in\mathbb{Z}_+$, is a root if

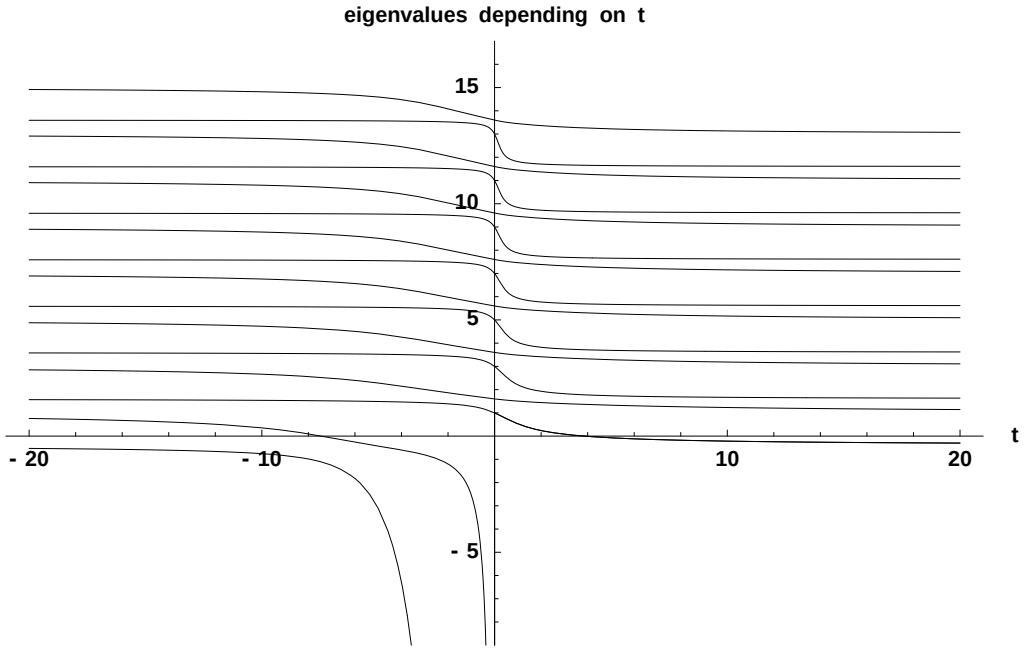

Figure 3.9: The Hamiltonian is determined by the boundary conditions corresponding to the parameters $(\xi, \eta, \zeta) = (0.95\,t, 0.25\,t, 0.25\,t)$, $\alpha = 0.3$, $B = 1$.

and only if $\xi = 0$, and finally $-\alpha - m$, with $m \in \mathbb{Z}_+$, is a root if and only if $\eta = 0$.

Let us note that this localization is in agreement with the following general result: if A and B are two self-adjoint extensions of the same symmetric operator with finite deficiency indices (d, d) then any interval $J \subset \mathbb{R}$ not intersecting the spectrum of A contains at most d eigenvalues of the operator B (including multiplicities) and no other part of the spectrum of B [W, §8.3]. Thus in our example if J is an open interval whose boundary points are either two subsequent eigenvalues of H^∞ or the lowest eigenvalue of H^∞ and $-\infty$ then any self-adjoint extension H^Λ has at most two eigenvalues in J.

3.4.6 Conclusion

A summary of the obtained results follows. The most general admissible family of Hamiltonians describing the system was properly defined. The operators were characterized by boundary conditions at the position of singularity. The spectrum of the standard Hamiltonian was defined explicitly, showing the splitting of the Landau levels and giving rise to finitely degenerated eigenvalues in each gap. The spectral properties of general Hamiltonians were investigated. Some particular cases were again solved explicitly. For the

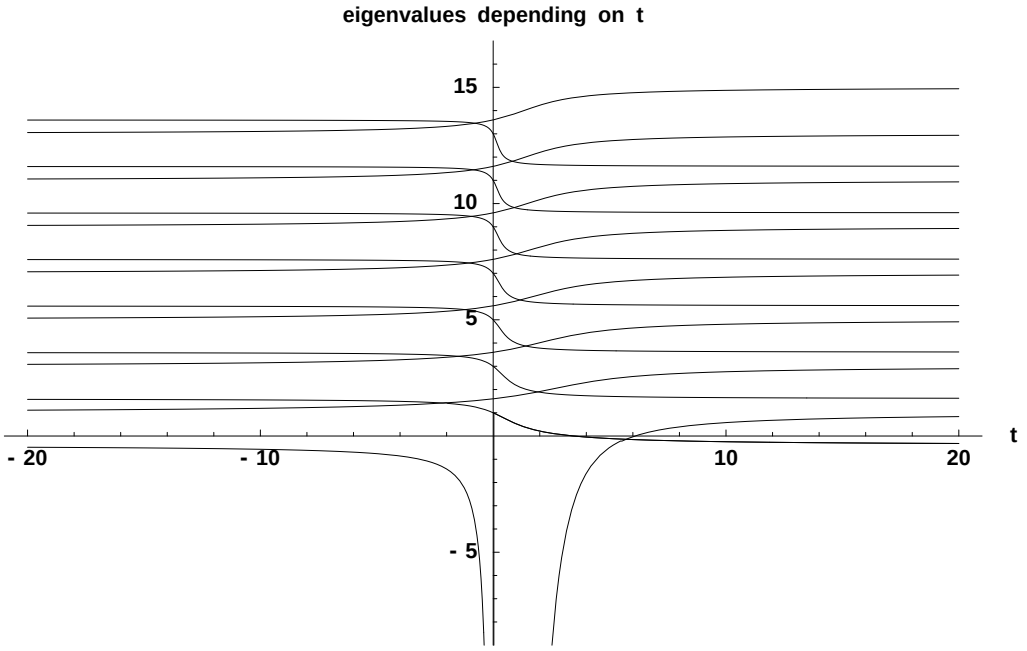

Figure 3.10: The Hamiltonian is determined by the boundary conditions corresponding to the parameters $(\xi, \eta, \zeta) = (0.95\,t, -0.25\,t, 0)$, $\alpha = 0.3$, $B = 1$.

general case, the number of newly arising eigenvalues was computed. The Green function for the standard Hamiltonian was found.

3.5 Further research

The purpose of this section is to show the article [EŠV] in a broader context of contemporary research. It is divided into two parts.

Section 3.5.1 is devoted to the noticeable work of Mine published in [M] where the generalization to more AB vortices is accomplished. Section 3.5.2 then gives a review of newer papers related to [EŠV] using its results or citing it, suggesting thus some directions where the study of similar topics is heading.

3.5.1 Generalization to the many solenoids problem

A natural generalization of the results of [EŠV] is contained in [M]. Therein, the system with homogeneous magnetic field and an arbitrary number (including the possibility of infinite amount) of idealized solenoids is considered.

All self-adjoint operators describing the system are found and completely characterized, and their spectral properties are studied. For finite quantity of solenoids, the bound on the number of eigenvalues between two neighbouring Landau levels (as well as below the lowest one) is provided. For a special case of sufficiently faraway points of singularities with uniform boundary conditions, the spectrum is localized in close vicinity of eigenvalues of some Hamiltonian with only one solenoid.

Preliminaries

Let us denote $\overline{\mathbb{N}} = \mathbb{N} \cup \{\infty\}$. The singularities are located in the points $\{z_j\}_{j=1}^N \subset \mathbb{R}^2,\ N \in \overline{\mathbb{N}}$ satisfying

$$R := \inf_{j \neq k} |z_j - z_k| > 0. \tag{3.49}$$

Then the positive symmetric operator L_N whose self-adjoint extensions describe the system is defined as

$$L_N = (-\imath\nabla + a_N)^2\,,$$
$$D(L_N) = C_0^\infty(\mathbb{R}^2 \setminus S_N).$$

Here $a_N \in C_0^\infty(\mathbb{R}^2 \setminus S_N) \cap L^1_{loc}(\mathbb{R}^2)$ are the potetials such that

$$\text{rot } a_n(z) = B + \sum_{j=1}^N 2\pi\alpha_j \delta(z - z_j)$$

in the distributional sense in $\mathcal{D}'(\mathbb{R}^2)$ for $z \in \mathbb{R}^2$, with $B > 0$ being the parameter of the field and $\alpha_j \in (0,1)\,\forall j \in N$ the parameters of the point interaction at the respective points z_j. The existence of such potentials was proven in [A1] and [A2].

The deficiency indices of L_N are proved to be $(2N, 2N)$. The self-adjoint extensions are denoted by H_N, and H_N^{AB} is the standard AB Hamiltonian.

Spectral properties

The results concerning the spectral properties of H_N are summarized in two main theorems.

Theorem 1.1. *Let $N \in \overline{\mathbb{N}}$ and let $P_I(H)$ denote the spectral projection of a self-adjoint operator H corresponding to an interval I and* $\text{mult}\{\lambda; H\} = \dim \text{Ker}(\lambda - H)$. *Then, the following holds:*
(i) For any self-adjoint extension H_N of L_N, we have

$$\text{mult}\{(2n-1)B; H_N\} = \infty, \quad n \in \overline{\mathbb{N}}.$$

(ii) For the Standard AB Hamiltonian H_N^{AB}, we have

$$\dim \mathrm{Ran}\, P_{(-\infty,B)}\left(H_N^{AB}\right) = 0,$$
$$\dim \mathrm{Ran}\, P_{((2n-1)B,(2n+1)B)}\left(H_N^{AB}\right) \leq nN, \quad n \in \overline{\mathbb{N}}.$$

(iii) For any self-adjoint extension H_N of L_N, we have

$$\dim \mathrm{Ran}\, P_{(-\infty,B)}\left(H_N\right) \leq 2N,$$
$$\dim \mathrm{Ran}\, P_{((2n-1)B,(2n+1)B)}\left(H_N\right) \leq (n+1)N, \quad n \in \overline{\mathbb{N}}.$$

This means that the infinite multiplicity of eigenvalues in Landau levels is always preserved. Moreover, there is no eigenvalue below the lowest Landau level for H_N^{AB} and at most $2N$ of them for arbitrary H_N, while between two Landau levels there are at most nN or $(n+1)N$ eigenvalues, respectively.

For the special case mentioned above, the notion of the operator with uniform boundary conditions has to be introduced. The definition uses the concept of magnetic translation operators defined in [Z].

Definition 1.2. *Let H_N be a self-adjoint extension of L_N. We say operator H_N has* uniform boundary conditions *if the following two conditions hold:*
(i) There exists $\alpha \in \mathbb{R}, 0 < \alpha < 1$ such that $\alpha_j = \alpha\ \forall j \in \widehat{N}$.
(ii) There exists a self-adjoint extension H_1 of L_1 independent of j such that

$$D(H_N) = \left\{ u \in D(L_N{}^*) \,\middle|\, t_{-z_j}(\chi_j u) \in D(H_1)\ \forall j \in \widehat{N} \right\}. \tag{3.50}$$

Here the condition (ii) says that the boundary conditions of H_N at the respective points z_j have to be equivalent to the boundary condition of H_1 at z. Thus functions from H_N have to be just a transformation of functions from $D(H_1)$, using the magnetic translation operators t_{-z_j}; here χ_j are some technical auxiliary functions.

Theorem 1.2. *Let $N \in \overline{\mathbb{N}}, N \geq 2$. Let H_N be a self-adjoint extension of L_N which has uniform boundary conditions and H_1 be the single solenoid operator appeared in (3.50). Let $I = [c,d]$ be a closed interval satisfying $I \cap \{(2n-1)B | n \in \overline{\mathbb{N}}\} = \emptyset$, $c, d \notin \sigma(H_1)$ and $\sigma(H_1) \cap I = \{\lambda_i\}_{i=1}^k$ (by Theorem 1.1, $\sigma(H_1) \cap I$ is a finite set).*

Then, there exist constants $u > 0$ and $R > 0$ dependent only on B, α, I and H_1 satisfying the following assertions:
(i) If $R \geq R_0$, we have

$$\sigma(H_N) \cap I \subset \bigcup_{l=1}^{k} |\lambda_l - \delta, \lambda_l + \delta|$$

where $\delta = e^{-uR^2}$.

(ii) If $R \geq R_0$*, we have*

$$\dim \mathrm{Ran}\, P_I(H_N) = N \dim \mathrm{Ran}\, P_I(H_1).$$

Recall that $R = \inf_{j \neq k} |z_j - z_k| > 0$ by (3.49).

Thus, in this large separation case, the eigenvalues of H_N differ from those of H_1 by δ at most. Moreover, there are exactly nN eigenvalues between the n-th and $(n+1)$-th Landau levels, i.e. the bound (iii) of Theorem 1.1 is reached. Together it means that the solenoids, provided the distances between them are sufficient, behave "independently" in some sense, and that the system is an intuitive generalization of the case with one solenoid with the respective boundary condition.

Theorem 1.1 is proven using a perturbation of the canonical commutation relation of the creation and anihilation operators corresponding to H_N^{AB}, and the proof of Theorem 1.2 follows a method used in [CN].

Characterization of self-adjoint extensions

In what follows, it is assumed that

$$(\exists \alpha_-, \alpha_+ \in \mathbb{R})(\forall j \in \widehat{N}, N \in \overline{\mathbb{N}})(\ 0 < \alpha_- \leq \alpha_j \leq \alpha_+ < 1\ ).$$

Moreover, a notation of operators with the upper index α (i.e. H_1^α) is introduced indicating explicitly the respective value of the flux.

An equivalent of the linear functionals (3.28) is formally introduced for the case of one solenoid. The operators $\Xi_j : D((L_1^{\alpha_j})^*) \setminus D(\overline{L_1^{\alpha_j}}) \to \mathbb{C}^4$ are defined by

$$\Xi_j[u] := (\Phi_{-1}^{\alpha_j}(u), \Psi_1^{\alpha_j}(u), \Phi_0^{\alpha_j}(u), \Psi_0^{\alpha_j}(u)), \quad [u] \in D((L_1^{\alpha_j})^*) \setminus D(\overline{L_1^{\alpha_j}})$$

for $j \in \widehat{N}$. Then, each operator $\Xi_j(u)$ returns the vector with four parameters of the self-adjoint extension (and thus those of the point interaction), computed for the singular part of the function u from the domain of an arbitrary self-adjoint extension $H_1^{\alpha_j}$; notice that $H_1^{\alpha_j} \subset (L_1^{\alpha_j})^*$.

Consequently, the generalization to the case with N singularities is implemented by defining the linear operator $\Xi : D(L_N{}^*) \setminus D(\overline{L_N}) \to \mathbb{C}^{4N}$ (with $\mathbb{C}^{4N} = l^2(\mathbb{N})$ for $N = \infty$) in the form

$$\Xi[u] := (\Xi_1[T_1 u], \ldots, \Xi_N[T_N u]).$$

Here T_j are some operators that enabled us to use the operators Ξ_j on singular parts of functions from $D(L_N{}^*)$ as well, bearing in mind that the singularities of L_1 and L_N are localized in different points in $\mathbb{R}^2$. Thus, in fact,

all the singular points are treated individually and compared to some one-solenoid extension $H_1^{\alpha_j}$. At the end, $\Xi(u)$ returns $4N$ (or infinitely many) parameters of point interactions corresponding to some Hamiltonian H_N, with $u \in D(H_N)$.

Using Ξ, a set of functions $\{\phi_{-1}^{(j)}, \psi_1^{(j)}, \phi_0^{(j)}, \psi_0^{(j)}\}$ is found that forms a basis of the deficiency subspace $D(L_N{}^*) \setminus D(\overline{L_N})$. Hence, the domain of $L_N{}^*$ is decomposed as

$$D(L_N{}^*) = D(\overline{L_N}) \oplus_{\text{alg}} \oplus_{j=1}^{N} [\phi_{-1}^{(j)}, \psi_1^{(j)}, \phi_0^{(j)}, \psi_0^{(j)}]_\lambda$$

where $\oplus_{\text{alg}}$ denotes the algebraic direct sum.

This allows the following characterization of self-adjoint extensions of L_n.

Theorem 5.11. *Let $N \in \overline{\mathbb{N}}$. Let M and J be bounded operators on $\mathbb{C}^{4N}$ satisfying*

$$\operatorname{Ran} M = \overline{\operatorname{Ran} M}, \qquad \operatorname{Ker} M^* J = \operatorname{Ran} M \tag{3.51}$$

and

$$J = \begin{pmatrix} J_{\alpha_1} & 0 & \dots & 0 \\ 0 & J_{\alpha_2} & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & J_{\alpha_N} \end{pmatrix}, \qquad J = 4\pi \begin{pmatrix} 0 & \alpha - 1 & 0 & 0 \\ 1 - \alpha & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -\alpha & 0 \end{pmatrix}.$$

Define an operator H_N^M by

$$\begin{aligned} D(H_N^M) &= \{u \in D(\overline{L_N}) \mid \Xi[u] \in \operatorname{Ran} M\}, \\ H_N^M &= (-\imath\nabla + a_N)^2 . \end{aligned}$$

Then, H_N^M is a self-adjoint extension of L_N. Moreover, for any self-adjoint extension H_N of L_N, there exists a bounded operator M on $\mathbb{C}^{4N}$ satisfying (3.51) and $H_N^M = H_N$.

In the case of one solenoid, this proposition is equivalent with the one of [EŠV]. Then, the following corollary holds true.

Corollary 5.12. *The map $M \mapsto H_N^M$ is a one-to-one correspondence between the set of the orthogonal projections M on $\mathbb{C}^{4N}$ satisfying* $\operatorname{Ker} MJ = \operatorname{Ran} M$ *and the set of the self-adjoint extensions H_N of L_N.*

A simplified version for special cases is provided as well.

Corollary 5.13. *(i) Let $N < \infty$. Then, the condition 3.51 is equivalent to*

$$\operatorname{rank} M = 2N, \quad M^* J M = 0,$$

where $\operatorname{rank} M = \dim \operatorname{Ran} M$.
(ii) Let $N \in \overline{\mathbb{N}}$. *Suppose that the operator* M *is the (finite or infinite) direct sum of* 4×4 *orthogonal projection matrices, that is,*

$$M = \begin{pmatrix} M_1 & 0 & \dots & 0 \\ 0 & M_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & M_N \end{pmatrix}, \qquad M_j : 4 \times 4,\ M_j^2 = M_j,\ M_j^* = M_j.$$

Then, the condition 3.51 is equivalent to

$$\operatorname{rank} M_j = 2, \quad M_j J_{\alpha_j} M_j = 0 \quad \forall j \in \widehat{N}.$$

3.5.2 Related and citing papers

A very brief review of some other papers related to our subject of interest and citing the article [EŠV] follows.

The planar system with a charged particle of spin 1/2 under the influence of two idealized AB fluxes is studied in [GŠ1], generalizing the setup with one solenoid. The self-adjoint extensions are found and characterized by boundary conditions at the points of singularity similar to those of [DŠ] and [EŠV]. The deficiency indices are found to be $(4, 4)$ and a basis of the deficiency subspace is derived using the knowledge of the spinless Green function. Finally, the Green function for the spin-1/2 case is constructed with the use of Krein's formula. The asymptotic analysis of functions near the singularity points is heavily used.

The articles [GGS2] and [GGS1] are a continuation of previous work of the authors, see references therein. They consider the relativistic case and study the Dirac equation in the so-called magnetic-solenoid field, denoting the combination of homogeneous magnetic field and flux due to the idealized AB effect. Self-adjoint extensions are found, and their spectral properties as well as boundary conditions are briefly investigated.

The time-dependent singular AB flux on the background of a homogeneous magnetic field is studied in [AHŠ2]. Here, the value of the flux is characterized by a C^2 monotonous function Φ instead of a real parameter. The adiabatic theorem is proven. A new theoretical concept has to be introduced, consisting in an association of a propagator to a time-dependent Hamiltonian in a weaker and more general way than in the standard case, however still preserving the uniqueness of this connection. The need for this new way was driven by the studied situation where the standard approach turned out to be impossible because of too strong requirements on the propagator.

In [RT], the systems with a homogeneous magnetic field perturbed by both magnetic and electric fields with compact support are considered. The spectral properties of corresponding Hamiltonians are studied, with focus on splitting of Landau levels. The approximate creation and annihilation operators are used and the asymptotics of the split eigenvalues is found under some conditions.

The work of [P] concerns a two-dimensional system with charged 1/2-spin particle and a homogeneous magnetic field with a compact support. Two specific extensions are compared. The Aharonov-Casher theorem (restricting the number of zero modes) is proved for one of them, while an approximation by regular fields is confirmed to be possible only for the other one, leaving the question of physical plausability unanswered.

The Dirac-Weyl operator for the homogeneous magnetic field and idealized AB effect was studied in [O].The deficiency indices are stated to be $(1, 1)$. The spectrum of the standard AB Hamiltonian is studied; no eigenvalue is found in the sector $m = -1$. The self-adjoint extensions are characterized by one parameter, and their spectrum is found.

There is an interest in systems with magnetic field and a AB fluxes placed in some periodic structures as well.

The two-dimensional system with a perpendicular homogeneous field and an arbitrary (finite or infinite) quantity of idealized AB fluxes with various periodic structures such as chains or lattices is considered in [GŠ1]. Zero modes, i.e. eigenfunctions corresponding to zero energy, are the subject of interest here, the main goal being to find conditions for their appearance. To do so, one version of the Aharonov-Casher ansatz is used. Then, the perturbations in the form of translation and addition of AB solenoids are addressed. Some consequences such as occurence of oscillations or absolute continuity of the spectrum are described.

There is a continuation of [M] in the work of Mine and Nomura concerning a homogeneous magnetic field with arbitrarily many idealized solenoids. In [MN1], periodically varying fluxes are investigated, while [MN2] concerns random δ magnetic fields. The conditions for having infinitely degenerated eigenvalues in Landau levels are given, and in the former case a possibility of occurance of purely continuous spectrum is stated. The spectral properties are studied.

Then some other physical situations were taken into consideration.

In [H4], the AB effect considered on a circle in two dimensions is investigated. A formal characterization of self-adjoint extensions is found.

The AB effect with its potential supported on a disc is studied in [BM]. Special interest is paid to the Fridrichs extension denoting the standard AB Hamiltonian. The corresponding parameters of the interaction are investi-

gated and the lowest eigenvalue is determined.

The paper [IY] considers system with AB effect on a punctured two-dimensional torus. Properties concerning both geometry and operator theory are investigated.

The particular self-extension with regular boundary condition describing the AB effect on the Poincaré disc, i.e. a hyperbolic disc pierced by an AB flux, is examined in [L3], with the aim to obtain the integral representation of wavefunctions and the resolvent kernel.

Chapter 4

Matter in strong magnetic fields

This chapter is devoted to the study of the H_2^+ molecule in strong magnetic fields. It is the presence of the fields that makes the existence of this otherwise unstable object possible. An explicitly solvable operator with point interactions is used as an approximation of the original Hamiltonian, and their convergence in resolvent norm sense is proved in high field limit. The basic properties of H_2^+ are investigated, including the stability and asymptotic behaviour of the ground state energy and the equilibrium distance. The results are summarized in two papers [BBjpa] and [BBfbs] that lie in the core of this part.

As to the structure of the text, we first introduce the notion of a strong magnetic field and mention some of its principal properties in Section 4.1. We explain in detail the approximative method used in the two papers in Section 4.2. In Section 4.3.1, we establish the systems describing the H_2^+. The review of the literature focused on strong magnetic fields in general and on H_2^+ molecule in particular is given in Section 4.4. Finally, the full text of papers [BBjpa] and [BBfbs] form the contents of Section 4.5.

4.1 Strong magnetic fields

Some basic remarks on strong magnetic fields will be made here. In Section 4.1.1, we describe for what values of magnetic field we talk about strong fields. A short description of change in the matter behaviour will be given in 4.1.2. Finally, some new functions used throughout the whole chapter will be introduced in 4.1.3

A detailed review of the literature about strong magnetic fields can be

found e.g. in [L2] and books [GHRW] and [SS].

Let us make a short remark about the notation here. Magnetic fields will be denoted by the symbol B (or some its modification such as $\mathbb{B}$, in some cases). The symbol H will be reserved for Hamilton operators. This is the standard notation in the literature concerning strong magnetic fields.

4.1.1 Definition

Shortly, a strong magnetic field is defined as a field of such strength that the cyclotron energy is much larger than the electrostatic energy needed to ionize a hydrogen atom, and for which the relativistic effect are negligible at the same time. The critical range of the field intensity where the conditions are fulfilled is

$$2.3505 \times 10^9 \text{ G} \ll B \lesssim 4 \times 10^{13} \text{ G}. \tag{4.1}$$

We first start with establishing the lower critical value. Let us consider an electron with mass m_e and charge e under the influence of a uniform magnetic field B. Then the cyclotron radius is

$$\rho = \left(\frac{\hbar c}{eB}\right)^{1/2}$$

and we have the cyclotron energy (and the distance between two adjacent Landau levels) as

$$\hbar\omega_{ce} = \hbar\frac{eB}{m_e c}.$$

The value B_0 is defined by setting the cyclotron radius equal to the Bohr radius, i.e. $\rho = a_0$, which leads to

$$B_0 = \frac{m_e^2 e^3 c}{\hbar^3} = 2.3505 \times 10^9 \text{ G},$$

giving the lower limit in (4.1). Equivalently, the critical value can be established by the requirement $\hbar\omega_{ce} = e^2/a_0$. Subsequently, a dimensionless magnetic field strength b can be introduced as

$$b = \frac{B}{B_0},$$

and the condition for strong fields reads $b \gg 1$.

From the other side, the upper limit is set up so as to prevent the relativistic effects from being significant. This happens for magnetic fields with

$\hbar\omega_{ce} \gtrsim m_e c^2$ where the transverse motion of the electron becomes relativistic, leading to the upper limit of (4.1) in the form

$$B_{rel} = \frac{m_e^2 c^3}{e\hbar} = \frac{B_0}{\alpha^2} = 4.414 \times 10^{13} \text{ G};$$

here $\alpha = e^2/\hbar c$ is the fine structure constant.

However, in [L2] it is argued that one can use the non-relativistic approach even for $B \gtrsim B_{rel}$. The justification for the claim is twofold. Firstly, the free electron energy is reduced to $E \simeq m_e c^2 + p_z^2/2m_e$ for the groundstates; thus, the electron remains nonrelativistic in the z-direction, i.e. along the field axis, provided that the binding energy E_B is much less than $m_e c^2$. Secondly, the shape of the Landau wavefunction is the same in both relativistic and nonrelativistic theory. Therefore, as long as $E_B/(m_e c^2) \ll 1$, the relativistic effect on bound states can be considered as a small correction according to [AD]. This way, it is possible to consider values of the field in the region

$$2.3505 \times 10^9 \text{ G} \ll B \lesssim 10^{16} \text{ G}.$$

With increasing density of the matter, this relativistic correction becomes more important.

4.1.2 Behavior of the matter

According to the definition of strong magnetic fields, the cyclotron energy (and thus the energy needed for jump to a higher Landau level) is much higher that the typical Coulomb energy needed to ionize the hydrogen atom. This leads to a massive qualitative change in the behavior of the matter.

Normally, magnetic effects can be treated as a perturbation to other (especially electrostatic) forces, an example being Zeeman splitting of a atomic energy levels. For $B \gg B_0$, however, the magnetic field itself starts to play a dominant role, and it is the Coulomb force that now has a perturbative character. The consequences are as follows.

Electrons in an atom first settle into the lowest Landau level as contrasted to normal situation whit gradual occupation of orbitals.

Atoms gain the structure of one-dimensional systems. The movement of the electrons in the directions perpendicular to the field is extremely confined, with $a_0 \gg \rho \sim B^{-1/2}$, and the electrostatic force bind the electrons along the magnetic field direction, which makes the atom to attain a narrow cylindrical shape.

Huge impact on the rules of matter stability is observed. Strong magnetic fields guarantee the stability of otherwise unstable system such as the

H_2^+ molecule. Moreover, the covalent bonding allows the needle-like atoms to form molecular chains along the field direction. Interactions between the linear chains can then lead to the formation of three-dimensional condensates. The question of formations of new atoms and molecules is discussed in literature. A short review of literature is contained in Section 4.4.

The depicted behavior changes apply primarily to individual atoms, molecules and zero-pressure condensed matter. With sufficiently high temperature or density of the medium, the effects of even the strong magnetic fields can vanish, see [L2, Section VI].

4.1.3 The Lambert function

Here we introduce some functions that will be used often throughout the Chapter 4. They will play an important role mainly when scaling operators with respect to the magnetic fields. In what follows, we will denote by $\alpha = \alpha(B)$ the unique positive solution of the equation

$$\alpha + \log \alpha = \frac{1}{2} \log B, \tag{4.2}$$

which is equivalent to $\alpha e^{\alpha} = \sqrt{B}$. Then, α can be written as

$$\alpha = W\left(\sqrt{B}\right),$$

where W is the principal branch of the Lambert function W (cf. [CGH$^+$]). The asymptotic behavior

$$\alpha = \frac{1}{2} \log B - \log^{(2)} B + \log 2 + O\left(\frac{\log^{(2)} B}{\log B}\right), \quad B \to \infty,$$

with $\log^{(2)}(x) = \log \log(x)$ will be interesting for us. Especially, we will use the fact that $\alpha \simeq \log(\sqrt{B})$ for $B \to \infty$.

4.2 Approximation by asymptotic models

This section is devoted to the method developed by Duclos and Brummelhuis, and published consequently in [BD1], [BD2] and [BD3].

We will explain the method on the example of atoms; however, its use is not limited to those. In this section, atoms with a general finite number of N electrons with spin are considered in $\mathbb{R}^3$. The Born-Oppenheimer approximation is used, and the mass of the nuclei is considered to be infinite. No

results concerning the case of finite nuclei mass (i.e. when this approximation is omitted) were published so far.

The method consists of a series of approximations of the original Hamiltonian by other three operators in high field limit.

One starts with the original Hamiltonian of the system in Section 4.2.1; it is called the exact operator (strictly speaking it is not exact as it already incorporates approximation about the fixed center of mass). Then a spectral decomposition with respect to the angular momentum is applied, and one restricts to some its fixed sector.

Subsequently three new Hamiltonians are derived in Section 4.2.2; they will be denoted h_{eff}, h_C and h_δ. These three Hamiltonians have a form of one-dimensional operators, albeit with the values in some vector space. We will see that they are good approximations since they converge to the exact Hamiltonian (restricted to fixed angular momentum sector) in the resolvent norm sense for intensity of the field going to infinity.

Finally, the convergence of these operators is established in the form of three theorems, including error bounds, in Section 4.2.3. The explanation contained in this section will closely follow [BD3].

The proofs of the convergence theorem of Section 4.2.3 is then sketched in Section 4.2.4. Some applications of the method are discussed in Section 4.2.5.

Let us make a short remark on terminology. The operators h_{eff}, h_C and h_δ will be given their individual names as effective Hamiltonian, Coulomb Hamiltonian and δ-Hamiltonian, respectively, upon their definitions in Section 4.2.2. However, when we will want to refer to all of them as to a group, we will use the term *asymptotical Hamiltonians* (due to their high-field convergence properties). We will use this notation in the further sections as well.

Further discussion about the method in the context of other literature, as well as its application to other than atomic systems, is contained in Section 4.4.

Throughout this section, we will work in the atomic units.

4.2.1 Spectral decomposition of the exact Hamiltonian

First one has to introduce the starting operator of the system.

The exact Hamiltonian

Let N be the number of electrons and let Z be the charge of the nuclei. The *exact Hamiltonian* $H^{\mathbb{S}}$ is defined as

$$H^{\mathbb{S}} = \sum_{j=1}^{N} \left(\frac{1}{2} \left(\frac{1}{i} \nabla_j - \frac{1}{2} \mathbb{B} \wedge r_j \right)^2 + \sigma_j \cdot \mathbb{B} - \frac{Z}{|r_j|} \right) + \sum_{1 \le j < k \le N} \frac{1}{|r_j - r_k|}. \quad (4.3)$$

Here subsequently $r_j = (x_j, y_j, z_j) \in \mathbb{R}^3$ denote the coordinates of the j-th electron, σ_j its spin, ∇_j the gradient with respect to r_j, and $\mathbb{B} = (0, 0, B)$ the magnetic field fixed in the z direction; one can take $B \ge 0$ without loss of generality. The spin z-component in the Pauli representation is given by

$$I \otimes \cdots \sigma_{z_j} \cdots \otimes I, \quad \sigma_{z_j} = \frac{1}{2} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix},$$

and acts on $\otimes_{i=1}^{N} \mathbb{C}^2$. By [KK], it is possible to establish $D(H^{\mathbb{S}})$ so that the operator $H^{\mathbb{S}}$ is essentially self-adjoint on the Hilbert space

$$\mathcal{H} = \bigoplus_{j=1}^{N} L^2(\mathbb{R}^3) \otimes \mathbb{C}^2.$$

To define physically relevant system describing the fermionic particles, one has to restrict $\mathcal{H}$ to the subspace of totally antisymmetric functions. This subspace is composed of functions $\psi(r_1, s_1, \ldots, r_N, s_N) \in L^2((\mathbb{R}^3 \times \{\pm 1\})^N)$ antisymmetric with respect to 4-tuples (r_j, s_j), with $s_j = \pm 1$ standing for spin up or down, respectively, of the j-th particle. Then σ_{z_j} acts as the multiplication operator by $s_j/2$.

It is then possible to get rid of the spin dependence of the operator. Since $H^{\mathbb{S}}$ commutes with spin operators σ_{z_j} for each j, it decomposes to a direct sum unitarily equivalent to

$$\bigoplus_{s_{z_j} \in \{\pm 1\}} \left(H^{\mathbb{S}}\big|_{\mathbb{S}_z = -NB/2} + \sum_{j=1}^{N} (1 + s_{z_j}) \frac{B}{2} \right),$$

with $\mathbb{S}_z = \sum_{j=1}^{N} \sigma_{z_j}$ standing for the z component of the total spin operator. Thus, it is possible to fix the spin of the electrons in their $s_{z_j} = -1$ states, and consider only

$$H = H^{\mathbb{S}}\big|_{\mathbb{S}_z = -NB/2}$$

acting on $\otimes_{j=1}^{N} L^2(\mathbb{R}^3)$ without loss of generality. The operator can be written as

$$H = H_0 + \mathcal{V}$$

with H_0 standing for the free Hamiltonian of mutually noninteracting particles, and $\mathcal{V}$ denotes the potential.

Spectral decomposition

In order to derive the asymptotic Hamiltonians, the spectral decomposition of H with respect to the angular momentum is necessary.

One starts with the free Hamiltonian. The operator H_0 of the system then reads

$$H_0 = \sum_{j=1}^{N} \frac{1}{2} \left(\left(\frac{1}{\imath} \nabla_{r_j} - \frac{1}{2} \mathbb{B} \wedge r_j \right)^2 - NB \right).$$

Since the electrons are independent, it is possible to express H_0 as a direct sum of N one-particle operators H_1 where

$$H_1 = \left(H_{osc} - \frac{B}{2} L_z \right) \otimes I_z + I_{x,y} \otimes \left(-\frac{1}{2} \partial_z^2 \right) - \frac{B}{2} \otimes I_{x,y,z},$$

with $L_z = -\imath x_j \partial_{y_j} + \imath y_j \partial_{x_j}$ being the angular momentum in the field direction, H_{osc} standing for the Hamiltonian of the harmonic oscillator

$$H_{osc} = -\frac{1}{2} \Delta_{x,y} + \frac{B^2}{8} \left(x^2 + y^2 \right),$$

and I_z, $I_{x,y}$, $I_{x,y,z}$ being the identity operators in corresponding coordinates.

Let moreover $\Pi_{m,n}$ acting on $L^2(\mathbb{R}^2)$ be the orthogonal projections in the x, y variables onto the one-dimensional subspaces spanned by $\chi_{m,n} \in L^2(\mathbb{R}^2)$, the normalized eigenfunctions of the operator $H_{osc} - B/2$ restricted to the eigenspace of L_z corresponding to the eigenvalue m. Then the spectral decomposition of H_1 has the form

$$H_1 = \bigoplus_{m \in \mathbb{Z}, n \in \mathbb{N}} \left(\frac{B}{2} (2n + |m| - m) - \frac{1}{2} \partial_z^2 \right) \mathbf{\Pi}_{m,n}$$

with the orthogonal projection $\mathbf{\Pi}_{m,n} = \Pi_{m,n} \otimes I_z$ acting on $L^2(\mathbb{R}^3)$.

Because of the simple structure of H_0 as a sum of the one-electron operators, one can write

$$H_0 = \bigoplus_{\mathbf{m} \in \mathbb{Z}^N, \mathbf{n} \in \mathbb{N}^N} \left[\sum_{j=1}^{N} \left(\frac{B}{2} \left(2n_j + |m_j| - m_j \right) - \frac{1}{2} \partial_{z_j}^2 \right) \right] \boldsymbol{\Pi}_{\boldsymbol{m},\boldsymbol{n}}$$

where $\boldsymbol{\Pi}_{\boldsymbol{m},\boldsymbol{n}}$ acting on $L^2(\mathbb{R}^{3N})$ are the eigenvector projections

$$\boldsymbol{\Pi}_{\boldsymbol{m},\boldsymbol{n}} = \mathbf{\Pi}_{m_1,n_1} \otimes \cdots \otimes \mathbf{\Pi}_{m_N,n_N}$$

labeled by N-tuples $\mathbf{m} = (m_i)_{i=1}^n \in \mathbb{Z}^N$ and $\mathbf{n} = (n_i)_{i=1}^n \in \mathbb{N}^N$.

The Lowest Landau Band of H_0 is defined as

$$\mathcal{L}_0 = \bigoplus_{\mathbf{m}\in\mathbb{N}_0^N} \operatorname{Ran} \mathbf{\Pi}_{\mathbf{m},\mathbf{0}}$$

where $\mathbf{0} = (0, \cdots, 0)$. Subsequently, let $F^{\mathbb{M}} = \mathcal{L}_0 \cap \operatorname{Ker}(\mathbb{L}_z - \mathbb{M})$ be the finite-dimensional space spanned by the lowest Landau states with total angular momentum $\mathbb{M}$, i.e.

$$F^{\mathbb{M}} = \bigoplus_{\mathbf{m}\in\Sigma(\mathbb{M})} \operatorname{Ran} \mathbf{\Pi}_{\mathbf{m},\mathbf{0}}$$

where

$$\Sigma(\mathbb{M}) = \left\{ \mathbf{m} = (m_i)_{i=1}^N \in \mathbb{N}_0^N \;\middle|\; \sum_{j=1}^N m_j = \mathbb{M} \right\}.$$

See the discussion at the end of the section for explanation of these restrictions.

Several simple observations can be made. The operator H_0 restricted to $\mathcal{L}_0$ equals to the free Laplacian Δ_z in the field direction. Denoting

$$X_{\mathbf{m}}(x, y) = \prod_{j=1}^N \chi_{m_j,0}(x_j, y_j), \quad m_1, \cdots, m_N \geq 0$$

(we recall that $\chi_{m_j,0}$ are the eigenfunctions of j-th oscillator Hamiltonian), then $\mathcal{L}_0$ is spanned by the tensor products $X_{\mathbf{m}} \otimes u$, with $u \in L^2(\mathbb{R}^N)$, and $X_m \otimes 1$ are generalized eigenvectors of H_0 with eigenvalue 0. The functions X_m are called lowest Landau band states.

The reduction of the Hamiltonians H and H_0 is then implemented, using the fact that both operators commute with the total orbital angular momentum in the field direction

$$\mathbb{L}_z = \sum_{j=1}^N \left(\frac{1}{\imath} x_j \partial_{y_j} - \frac{1}{\imath} y_j \partial_{x_j} \right).$$

Let $P^{\mathbb{M}}$ be the orthogonal projection onto the $\mathbb{M}$-th eigenspace of $\mathbb{L}_z$, with $L_{z_j} = m_j$ and $\sum_{j=1}^N m_j = \mathbb{M} \in \mathbb{N}_0$. One then defines the operators

$$H^{\mathbb{M}} = H P^{\mathbb{M}}, \qquad H^{\mathbb{M}} = H_0 P^{\mathbb{M}}$$

acting on $L^2(\mathbb{R}^{3N})$.

The *effective projection* $\Pi_{\text{eff}}^{\mathbb{M}}$ is defined as the orthogonal projection onto $F^{\mathbb{M}}$, and it reads

$$\Pi_{\text{eff}}^{\mathbb{M}} = \sum_{\mathbf{m}\in\Sigma(\mathbb{M})} \mathbf{\Pi}_{\boldsymbol{m},\mathbf{0}}. \tag{4.4}$$

The complementary projection $\Pi_{\perp}^{\mathbb{M}}$ is then the orthogonal projection on $\mathrm{Ran}(\Pi_{\mathrm{eff}}^{\mathbb{M}})^{\perp} \cap \mathrm{Ran}(P^{\mathbb{M}})$, i.e.

$$\Pi_{\perp}^{\mathbb{M}} = I - \Pi_{\mathrm{eff}}^{\mathbb{M}} = \sum_{\substack{\mathbf{m}\in\Sigma(\mathbb{M}) \\ \sum_j n_j \geq 0}} \boldsymbol{\Pi}_{\boldsymbol{m},\boldsymbol{n}}. \tag{4.5}$$

Let us note that $\mathrm{Ran}\,\Pi_{\mathrm{eff}}^{\mathbb{M}}$ can be identified with the space $L^2(\mathbb{R}^N, F^{\mathbb{M}})$ of $F^{\mathbb{M}}$-valued L^2-functions.

Moreover, it is important to realize that $H^{\mathbb{M}}$, $\Pi_{\mathrm{eff}}^{\mathbb{M}}$, $F^{\mathbb{M}}$ and other objects depend explicitly on both $\mathbb{M}$ and B.

Fixing of the angular momentum sector

As mentioned above, the restriction is made with respect to the value of the total angular momentum in the field direction $\mathbb{M}$. The rationale for that step is as follows.

The subject of our main interest is the spectral behavior of H near its lowest energy levels. Therefore, it is possible to consider only those sectors of angular momentum for which that occurs. This in turn leads to the restriction on $\mathbb{M}$ to the values from $\mathbb{N}_0$ because $\mathcal{L}_0 \cap \mathrm{Ran}\, P^{\mathbb{M}} \neq \{0\} \Leftrightarrow \mathbb{M} \geq 0$. Since $H^{-\mathbb{M}}$ is unitarily equivalent to $H^{\mathbb{M}} + \mathbb{M}B$, it holds true that $\inf \sigma(H^{\mathbb{M}\geq 0}) < \inf \sigma(H^{\mathbb{M}<0})$ for every $B > 0$.

The choice $\mathbf{n} = \mathbf{0}$ is driven by the same reason.

For justification of this fixing, see the discussion in Section 4.4.

Remark on notation Thus from now on, we will always consider $\mathbb{M} \geq 0$ fixed and work only in the corresponding sector.

For the sake of simplicity, we will omit the upper index $^{\mathbb{M}}$ in the following text. So from now on, we write H instead of $H^{\mathbb{M}}$, H_0 instead of $H_0^{\mathbb{M}}$, and the same for $\Pi_{\mathrm{eff}}^{\mathbb{M}}$, $\Pi_{\perp}^{\mathbb{M}}$, $F^{\mathbb{M}}$ an so forth, unless otherwise stated. Bear in mind that this will apply to newly defined objects as well – while they will be mostly restricted to the sector $\mathbb{M}$, the corresponding index will be suppressed.

4.2.2 Asymptotic Hamiltonians

The definitions of the three asymptotic Hamiltonians, serving for an approximative description of the system for large B, will be provided here. Their respective convergence theorems, showing precisely the character of this approximation, will be stated later in Section 4.2.3.

The effective Hamiltonian

The *effective Hamiltonian* h_{eff} is defined as the restriction of H to the lowest Landau level with fixed value of angular momentum $\mathbb{M}$ by the relation

$$h_{\text{eff}} = \Pi_{\text{eff}}\, H\, \Pi_{\text{eff}}.$$

It acts on Hilbert space $\operatorname{Ran}\Pi_{\text{eff}} = \Pi_{\text{eff}}\mathcal{H}$ that depends explicitly on B and $\mathbb{M}$, and is isomorhpic to the space $L^2(\mathbb{R}^N, F)$. One can get rid of the B-dependence of $\operatorname{Ran}\Pi_{\text{eff}}$ by rescaling; this is in fact used in the process of deriving the other asymptotic operators.

The potential term of h_{eff},

$$\mathcal{V}_{\text{eff}} = \Pi_{\text{eff}}\mathcal{V}\Pi_{\text{eff}},$$

can be interpreted as an operator valued function of $z = (z_1, \cdots, z_N) \in \mathbb{R}^N$, with values in the space of linear operators on $F^{\mathbb{M}}$ and acting in the natural way on $L^2(\mathbb{R}^N_z, F)$.

It is thus possible to consider the effective operator h_{eff} as one-dimensional multi-particle Schrödinger operator on the real line in variable z, and write

$$h_{\text{eff}} = -\frac{1}{2}\Delta_z - Z\sum_j V_j(z_j) + \sum_{j<k} V_{jk}(z_j - z_k). \tag{4.6}$$

Here the potentials V_j correspond to the interaction between the electron and the nuclei, while V_{jk} correspond to inter-electron interactions. They are defined by projecting the respective Coulomb potentials in (4.3) along Π_{eff},

$$V_j(z_j) = \Pi_{\text{eff}}\frac{1}{|r_j|}\Pi_{\text{eff}}$$
$$V_{jk}(z_j - z_k) = \Pi_{\text{eff}}\frac{1}{|r_j - r_k|}\Pi_{\text{eff}}.$$

By examining of the asymptotic behavior of these potentials for $B \to \infty$, the potentials of the other asymptotic Hamiltonians are found.

We now introduce

$$\overline{h}_{\text{eff}} = h_{\text{eff}} \otimes I_F$$

with I_F being the identity on F. Finally, it is convenient to complete h_{eff} as follows

$$H_{\text{eff}} = h_{\text{eff}} \oplus H_\perp$$

where

$$H_\perp = \Pi_\perp H \Pi_\perp$$

is the orthogonal complement of h_{eff}. The operator H_{eff} appears later in the convergence theorem.

The Coulomb Hamiltonian

Based on the behavior of the potential of the operator h_{eff} for large B as described later in Section 4.2.4, the second asymptotic Hamiltonian will be established here. For this, we need to define the tempered distribution q on $\mathbb{R}$ as

$$q(z) = \log B\ \delta(z) + \text{Pf}\ \left(\frac{1}{|z|}\right). \tag{4.7}$$

Here

$$\text{Pf}\left(\frac{1}{|z|}\right) = \frac{\mathrm{d}}{\mathrm{d}x}\left(\text{sgn}(z)\log|z|\right)$$

is the finite part of the singular function $1/|z|$ that regularizes the Coulomb potential from (4.3) on the line; the derivative is considered in distributional sense here. Then the finite-dimensional operators

$$C_j = -\Pi_{\text{eff}} \log\left(\frac{B}{4}(x_j^2 + y_j^2)\right)\Pi_{\text{eff}}$$

and

$$C_{jk} = -\Pi_{\text{eff}} \log\left(\frac{B}{4}\left((x_j - x_k)^2 + (y_j - y_k)^2\right)\right)\Pi_{\text{eff}},$$

both acting on $L^2(F)$, are introduced, stemming from the potentials corresponding to the electron-nuclei and inter-electron interactions, respectively.

The *Coulomb Hamiltonian* acting on $L^2(\mathbb{R}^N, F)$ is formally defined by

$$\begin{aligned} h_C = &-\frac{1}{2}\Delta_z - Z\sum_j \left(q(z_j) + C_j\delta(z_j)\right) \\ &+ \sum_{j<k}\left(q(z_j - z_k) + C_{jk}\delta(z_j - z_k)\right), \end{aligned} \tag{4.8}$$

the potential being denoted as v_C. Let us note that the δ and q are the first two terms in asymptotic expansion of the effective potential; they have zero-range and long range character, respectively. In q, the part $\text{PF}(1/z)$ influences the electron motion in the field direction, while C_j and C_{jk} in the transversal directions.

It is then necessary to provide a rigorous definition of h_C as a self-adjoint operator. Let $\langle\cdot,\cdot\rangle$ denote the duality between distributions and test functions, and let $(\cdot,\cdot)$ be the inner product on F. Moreover, let $L_j, L_{jk} : \mathbb{R}^N \to \mathbb{R}$ be linear maps such that $L_j(z) = z_j$ and $L_{jk}(z) = z_j - z_k$, and introduce

$$t_C(u) = \frac{1}{2}||\nabla u||^2 - Z\sum_j \left\langle L_j^* q,\ |u|^2 \right\rangle + \left\langle (L_j^*\delta,\ (C_j u, u) \right\rangle + \sum_{j<k} \left\langle L_{jk}^* q,\ |u|^2 \right\rangle + \left\langle L_{jk}^*\delta,\ (C_{jk}u, u) \right\rangle . \tag{4.9}$$

It can be proven that t_C is a well-defined quadratic form on the Sobolev space $H^1(\mathbb{R}^N, F)$, and that it is bounded from below by $-C||u||^2$, with C being some constant depending on B, Z, N and $\mathbb{M}$. By the Kato-Lax-Lions-Milgram-Nelson Theorem (cf. e.g. [RS1, Theorem X.17]), t_C defines a unique self-adjoint operator h_C. The characterization of the operator domain of h_C is provided in Theorem A.1 in [BD3].

Analogically to the effective case, the operator

$$H_C = \overline{h}_C \oplus H_\perp$$

appearing in the convergence theorem is established, with $\overline{h}_C = h_C \otimes I_F$.

We make only a short note concerning the potentials in h_C and their relation to the asymptotic expansion of the original Coulomb potential in H for $B \to \infty$. The first order term in this expansion equals to the zero-range δ-interactions appearing in h_C. The second order term has two parts describing the long range interactions in both magnetic and transversal directions; they are represented by Pf $(|z|^{-1})$ and C_j, C_{jk}, respectively.

The δ-Hamiltonian

From the operator h_C, the last asymptotic Hamiltonian can be derived. The *delta-Hamiltonian* acting on $L^2(\mathbb{R}^N, F)$ is defined as

$$h_\delta = -\frac{1}{2}\Delta_z + 2\alpha(B)v_\delta$$

with the potential

$$v_\delta(z) = -Z\sum_{j=1}^N \delta(z_j) + \sum_{j<k} \delta(z_j - z_k); \tag{4.10}$$

recall that α is defined in (4.2). As can be seen, h_δ is a simplified version of the Coulomb Hamiltonian h_C, with v_δ preserving only the (modified) leading term in the potential of h_C. Contrary to the original coupling constant $\log B$ of (4.7), its counterpart in h_δ is chosen to be $2\alpha(B)$, the reasons for that

being smaller error estimates arising in the convergence theorem and the fact that, unlike with $\log B$, we have $2\alpha(B) > 0$ for all $B > 0$.

While the Hilbert space h_δ acts on depends on $\mathbb{M}$, the operator itself is $\mathbb{M}$-independent, in contrast with the asymptotic Hamiltonians h_{eff} and h_C. The self-adjointness of the operator is established in the same manner as with the Coulomb Hamiltonian.

Once again, we set

$$H_\delta = \overline{h}_\delta \oplus H_\perp$$

with $\overline{h}_\delta = h_\delta \otimes I_F$.

4.2.3 Convergence theorems

This subsection contains the results of the method in the form of convergence theorems for the asymptotic Hamiltonians h_{eff}, h_C and h_δ (or better, for their complete counterparts H_{eff}, H_C and H_δ) defined in Section 4.2.2. The differences in the bounds can be seen for each version.

It is important to emphasize that we still consider $\mathbb{M} \geq 0$ fixed. Thus we should always bear in mind that $H_{\text{eff}} = H_{\text{eff}}^{\mathbb{M}}$, $H_C = H_C^{\mathbb{M}}$, $H_\delta = H_\delta^{\mathbb{M}}$, and so forth.

The effective Hamiltonian

The convergence theorem for the effective Hamiltonian has the following form.

Theorem 1.1. *For $\xi \in \mathbb{R}$ denote $d_{\text{eff}} = \operatorname{dist}(\xi, \sigma(h_{\text{eff}}))$. Then there exist positive constants B_{eff}, c_{eff} and C_{eff}, which only depend on Z, N and $\mathbb{M}$, such that for all $B \geq B_{\text{eff}}$, and all $\xi \in \mathbb{R}$ satisfying*

$$c_e f \frac{\alpha}{\sqrt{B}} \leq d_{\text{eff}} \leq \frac{1}{2}\alpha^2,$$

we have that $\xi \in \rho(H)$, and

$$\left\|(H-\xi)^{-1} - (H_{\text{eff}}-\xi)^{-1}\right\| \leq C_{\text{eff}} \frac{\alpha(B)^2}{d_{\text{eff}}^2\sqrt{B}}.$$

It can be shown that $\sigma(h_{\text{eff}}) = \sigma(H_{\text{eff}})$ for $B \geq B_{\text{eff}}$.

The Coulomb Hamiltonian

The convergence theorem for the Coulomb Hamiltonian has the following form.

Theorem 1.3. *For $\xi \in \mathbb{R}$ denote $d_C = \operatorname{dist}(\xi, \sigma(h_C))$. Then there exists positive constants B_C, c_C and C_C which depend only on Z, N and $\mathbb{M}$, such that for all $B \geq B_C$ and all $\xi \in \mathbb{R}$ satisfying*

$$c_C \frac{\alpha^{3/2}}{B^{1/4}} \leq d_C \leq \frac{1}{4}\alpha^2,$$

we have that $\xi \in \rho(H)$, and

$$\left\|(H-\xi)^{-1} - (H_C - \xi)^{-1}\right\| \leq \frac{C_C \alpha^{3/2}}{B^{1/4} d_C^2}.$$

The δ-Hamiltonian

The convergence theorem for the δ-Hamiltonian has the following form.

Theorem 1.5. *For $\xi \in \mathbb{R}$ denote $d_\delta = \operatorname{dist}(\xi, \sigma(h_\delta))$. Then there exist positive constants B_δ, c_δ and C_δ, depending on N, Z and $\mathbb{M}$, such that for all $B \geq B_\delta$ and $\xi \in \mathbb{R}$ satisfying*

$$c_\delta \alpha \leq d_\delta \leq \frac{1}{4}\alpha^2, \tag{4.11}$$

we have that $\xi \in \rho(H^{\mathbb{M}})$, and

$$\left\|(H-\xi)^{-1} - (H_\delta - \xi)^{-1}\right\| \leq \frac{C_\delta \alpha}{d_\delta^2}.$$

4.2.4 Proofs of the convergence theorems

The proofs of the convergence theorems consist of a sequence of estimates leading first to the result for the effective Hamiltonian, and from that to the Coulomb and delta- models. Since the machinery is technically quite complicated, only the main principles will be sketched, and many technical assumptions and results will be omitted.

For the sake of lucidity and ease of reference, the various constants emerging from the bounds will be denoted in the same way as they were established in [BD3].

The Feschbach decomposition

The first step is the decomposition of H to its effective part and the rest that will vanish in the limit. To this aim, some new notation is necessary. Once again, it is important to stress that fixed $\mathbb{M} \geq 0$ is considered throughout the subsection. Therefore, almost all new operators defined here should be considered as having the $^{\mathbb{M}}$ index, i.e. being restricted to some fixed angular momentum sector.

As said, he Hamiltonian H (now considered in the sector $\mathbb{M}$ of $\mathbb{L}_z$) is written as

$$H = H_0 + \mathcal{V}$$

with

$$\mathcal{V} = -\sum_j \frac{Z}{|r_j|} + \sum_{j<k} \frac{1}{|r_j - r_k|},$$

being the potential, and we introduce

$$T = H_0 P^{\mathbb{M}}, \quad T_{\text{eff}} = \Pi_{\text{eff}} T \Pi_{\text{eff}}, \quad T_\perp = \Pi_\perp T \Pi_\perp.$$

Then we make use of the projectors Π_{eff}, $\Pi_\perp$ established in (4.4) and (4.5), and denote as

$$\begin{aligned} \mathcal{V}_{\text{eff}} &= \Pi_{\text{eff}} \mathcal{V} \Pi_{\text{eff}}, & \mathcal{V}_\perp &= \Pi_\perp \mathcal{V} \Pi_\perp, \\ \mathcal{V}_{\perp,\text{eff}} &= \Pi_\perp \mathcal{V} \Pi_{\text{eff}}, & \mathcal{V}_{\text{eff},\perp} &= \Pi_{\text{eff}} \mathcal{V} \Pi_\perp, \\ H_{\perp,\text{eff}} &= \Pi_\perp H \Pi_{\text{eff}}, & H_{\text{eff},\perp} &= \Pi_{\text{eff}} H \Pi_\perp. \end{aligned}$$

operators acting respectively on $\operatorname{Ran} \Pi_{\text{eff}}$, $\operatorname{Ran} \Pi_\perp$, and between them. Then the resolvent-like operators

$$\begin{aligned} R &= (H_\perp - \xi)^{-1}, \\ R^{\mathcal{W}}_{\text{eff}} &= (h_{\text{eff}} + \mathcal{W} - \xi)^{-1}, \end{aligned}$$

are defined, with

$$\mathcal{W} = -\mathcal{V}_{\text{eff},\perp} R \mathcal{V}_{\perp,\text{eff}};$$

notice that they all depend explicitly on the spectral parameter ξ.

Then one can finally introduce the above mentioned decomposition and write H as

$$H = \begin{pmatrix} h_{\text{eff}} & H_{\text{eff},\perp} \\ H_{\perp,\text{eff}} & H_\perp \end{pmatrix} = \begin{pmatrix} T_{\text{eff}} + \mathcal{V}_{\text{eff}} & \mathcal{V}_{\text{eff},\perp} \\ \mathcal{V}_{\perp,\text{eff}} & T^B_\perp + \mathcal{V}_\perp) \end{pmatrix}.$$

In order to compare the resolvents, the Feschbach formula is used to give

$$(H - \xi)^{-1} = \begin{pmatrix} R^{\mathcal{W}}_{\text{eff}} & -R^{\mathcal{W}}_{\text{eff}} \mathcal{V}_{\text{eff},\perp} R \\ -R \mathcal{V}_{\perp,\text{eff}} R^{\mathcal{W}}_{\text{eff}} & R + R \mathcal{V}_{\perp,\text{eff}} R^{\mathcal{W}}_{\text{eff}} \mathcal{V}_{\text{eff},\perp} R \end{pmatrix} \tag{4.12}$$

for those $\xi \in \mathbb{C}$ for which the right hand side makes sense. After a series of bounds on all operators on the RHS of (4.12) one arrives to the formula

$$\left\|(H-\xi)^{-1} - (h_{\text{eff}} + \mathcal{W} - \xi)^{-1} \oplus R\right\| \leq \frac{C_{(37)}}{d_{\text{eff}}^{\mathcal{W}}\sqrt{B}} \tag{4.13}$$

for some $C_{(37)}$ and $d_{\text{eff}}^{\mathcal{W}}$.

Asymptotic potentials for large fields

The behavior of the potential h_{eff} is then studied for large values B of magnetic fields, leading to the other asymptotic potentials v_C and h_δ of the corresponding Hamiltonians.

One starts with the operator h_{eff} and eliminates the B-dependence from the Hilbert space $L^2(R^N, F)$ it acts on (more concretely, from the only part F that depends on B), by using some unitary rescaling of the operators with respect to B. This leads to some unitarily equivalent space $L^2(R^N, F_1)$. Moreover, it means that the modified potentials V_j^1, V_{jk}^1 gains independence of B as well (the B-dependence of original potentials V_j, V_{jk} stemmed from sandwiching by projectors Π_{eff}), and it is possible to write

$$h_{\text{eff}} = -\frac{1}{2}\Delta_z - Z\sum_j \sqrt{B}V_j^1(\sqrt{B}z_j) + \sum_{j<k}\sqrt{B}V_{jk}^1(\sqrt{B}(z_j - z_k)).$$

Then the following fact is used. Define $R_0 = \left(\frac{1}{2}\Delta_z - \beta^2\right)^{-1}$ for some spectral parameter β. If u is a function or tempered distribution $\mathbb{R}^N \to F$, then $\|R_0^{1/2}u\|_{L^2(\mathbb{R}^N,F)}$ is a norm on the 1st Sobolev space $H^1(\mathbb{R}^N F)$. A linear operator A sends $H^1(\mathbb{R}^N, F)$ continuously into $H^{-1}(\mathbb{R}^N, F)$ if and only if the L^2-operator norm $\|R_0^{1/2}AR_0^{1/2}\|$ is finite.

By controlling this norm for various distributions, it is possible to show that the potentials V_j, V_{jk} from (4.6), v_δ from (4.10), and the parts q, δ, C_j and C_{jk} from (4.8) are well defined. This allows to establish the potential v_C and leads to introduction of h_C and h_δ as of a self-adjoint operators as described in Subsection 4.2.2.

Bound on resolvents of the asymptotic Hamiltonians

Subsequently, it is necessary to eliminate the term $\mathcal{W}$ from (4.13). Using symmetrized resolvent formula, $\|R_0^{1/2}AR_0^{1/2}\|$-type estimates and some other computations one can arrive at the bound

$$\left\| R_{\text{eff}}^{\mathcal{W}}(\xi) - r_{\text{eff}}(\xi)\right\| \leq c_{\text{eff}}\frac{\alpha}{{d_{\text{eff}}}^2\sqrt{B}} \tag{4.14}$$

for some c_{eff}, with d_{eff} defined in Theorem 1.1.

Finally, by combining (4.13) and (4.14) one can prove the convergence theorem for the effective Hamiltonian, with the constant C_{eff} therein being computed from c_{eff}, $c_{(37)}$ and further constants coming from the other bounds.

Having the theorem for the effective Hamiltonian is the keystone for transition to both Coulomb and delta Hamiltonians, as it suffices to find the bound between h_{eff} and h_C (or h_δ, respectively).

The steps to the Coulomb and δ-models are quite straightforward. Using again the symmetrized resolvent formula and similar arguments as in the case of h_{eff} it is possible to arrive at the analogues of (4.14), namely

$$\|r_{\text{eff}}(\xi) - r_C(\xi)\| \leq C'_C \frac{\alpha^{3/2}}{d_C^2 B^{1/4}} \tag{4.15}$$

and

$$\|r_{\text{eff}}(\xi) - r_\delta(\xi)\| \leq C'_\delta \frac{\alpha}{{d_\delta}^2}, \tag{4.16}$$

again for some C'_C, d_C defined in Theorem 1.3, and $C'\delta$, d_δ defined in Theorem 1.5, respectively. The convergence theorems for the Coulomb and δ-Hamiltonians (and all respective constants) are derived by combining (4.15) and (4.16) with the theorem for the effective model.

4.2.5 Application of the results

We describe one potential application of the depicted method, namely an approximation of the spectrum of the exact Hamiltonian.

Let $E_\delta = \inf h_\delta$ be a simple isolated eigenvalue of h_δ. Then for sufficiently large B, the exact operator H has a set of eigenvalues with total multiplicity equal to $\dim F$ in the interval $(E_\delta - c_\delta\alpha^2, E_\delta + c_\delta\alpha^2)$, with c_δ defined in (4.11) in Theorem 1.5. Moreover, for the special case when $\dim F = 1$, the relation $\|\Psi - \Psi_\delta\|_{L^2(\mathbb{R}^{3N})} = O(\alpha^{-1}), B \to \infty$ holds true for the corresponding eigenvector Ψ of H, and for $\Psi_\delta(x, y, z) = \varphi_\delta(z)X_{\mathbf{m}}(x, y)$ with φ_δ being the corresponding eigenvector of h_δ.

The rationale of the claim is quite simple. For $B > B_\delta$, it is known that $\sigma(H_\delta) \subset (0, \infty)$ from Theorem 1.5. Therefore, it has to be $E_\delta < 0$. If E_δ is an eigenvalue of h_δ, then at the same time, E_δ is an eigenvalue of $H_\delta = h_\delta \oplus H_\perp$ with multiplicity of $\dim F$. Let Γ be the circle in the complex plane centered at E_δ with radius $c_\delta\alpha^2$. Moreover, let P and P_δ be the eigenprojections onto the spectra $\sigma(H)$ and $\sigma(h_\delta)$, respectively, inside Γ. Then for $B > B_\delta$, it is possible to prove that $\dim P = \dim P_\delta = \dim F$ which leads to the conclusion above.

4.3 Molecule H_2^+

This section will be devoted to the definition the physical system that is investigated in [BBjpa] and [BBfbs]. We introduce the Hamiltonian of the exact system as well as a one-dimensional asymptotic operator with singular potential that serves as its approximation. Literature concerning this system will be discussed in Section 4.4.

4.3.1 The system

The H_2^+ molecule consists of two nuclei and one non-relativistic electron considered in $\mathbb{R}^3$. The magnetic field is oriented in the z-direction, and both the nuclei are aligned along the z-axis as well. We begin by establishing the Hamiltonian of the system.

The exact Hamiltonian

Let subsequently $r = (x, y, z) \in \mathbb{R}^3$ be the coordinates of the electron, $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ the electron spin vector, $R = |R_1 - R_2|$ the inter-nuclear distance, with the nuclei being located at $R_1, R_2 \in \mathbb{R}$ on the z-axis, $Z = (Z_1, Z_2)$ the charges of the nuclei, and $\mathbb{B} = (0, 0, B)$ the magnetic field fixed in the z direction; we can take $B \geq 0$ without loss of generality. The Born-Oppenheimer approximation is considered. Then the Pauli Hamiltonian of the system reads

$$H = \frac{1}{2}\left(\frac{1}{i}\nabla - \frac{1}{2}\mathbb{B} \wedge r\right)^2 + \sigma \cdot \mathbb{B} - V + \frac{Z_1 Z_2}{R}, \tag{4.17}$$

where V is the electron-nuclei potential

$$V(r) = \frac{Z_1}{|r - R_1 z|} + \frac{Z_2}{|r + R_2 z|}$$

and the term $Z_1 Z_2 / R$ corresponds to the interaction between the nuclei. Operator (4.17) acts on $L^2(\mathbb{R}^3)$, and is the H_2^+-equivalent of the exact Hamiltonian $H^{\mathbb{S}}$ from (4.3).

The special homonucleus situation is often considered, with $Z = Z_1 = Z_2 > 0$ and $-R_1 = R_2 = R/2$.

The δ-model

To model the explicitly unsolvable system (4.17), new Hamiltonians using the zero-range δ-potentials instead of the original Coulomb potentials were proposed in the literature, see Section 4.4 for a more detailed discussion.

The most frequently used δ-Hamiltonian formally reads

$$h_\delta = -\frac{1}{2}\frac{d^2}{dx^2} - Z_1\delta_{R_1} - Z_2\delta_{R_2} + \frac{Z_1 Z_2}{R} \tag{4.18}$$

with $\delta_{R_i}(x) = \delta(x - R_i), i = 1, 2$, being the one-dimensional singular-potential counterpart of the exact operator (4.17) introduced above. The special homonucleus variant appears often as well.

In order to deal with the singular potentials in (4.18) and define the operator h_δ rigorously as an operator acting on $L^2(\mathbb{R})$, one can set

$$\begin{aligned} h_\delta =& -\frac{d^2}{dx^2}, \\ D(h_\delta) =& \Big\{ \psi \in H^{2,1}(\mathbb{R}) \cap H^{2,2}(\mathbb{R} \setminus \{R_1, R_2\}) \Big| \\ & \lim_{r \downarrow 0} (\psi'(R_i + \varepsilon) - \psi'(R_i - \varepsilon)) = 2Z_i \psi(R_i), i = 1, 2 \Big\}. \end{aligned} \tag{4.19}$$

We recall that the model defined here can be regarded as just a special case of the more general operator established in 2.4. The boundary condition in (4.19) ensures that h_δ is self-adjoint (cf. [AGHKH1]), and that it is uniquely associated to the quadratic form

$$\begin{gathered} q_\delta(\phi, \psi) = \frac{1}{2}\langle \phi', \psi' \rangle - \sum_{i=1}^{2} Z_i \overline{\phi}(R_i)\psi(R_i) \\ D(q_\delta) = H^{2,1}(\mathbb{R}). \end{gathered}$$

The quadratic form is densely defined, closed and semibounded. Contrary to h_δ, the domain of q_δ does not depend on Z and R.

Alternatively to (4.18), an re-scaled operator is used often. Here, we will present it in the special homonucleus case with $Z = Z_1 = Z_2 > 0$ and $-R_1 = R_2 = R/2$. Then we have

$$h_\delta = L^2 Z^2 \left(\frac{1}{2}\frac{d^2}{dx^2} - \delta(z - a) - \delta(z - a) \right) + \frac{Z^2}{R},$$

where $a = RLZ/2$.

Basic spectral properties

Several observation about the spectrum of h_δ can be made based on the general results, e.g. [AGHKH1, Theorem 2.1.3].

It holds true that $\sigma_{\mathrm{ess}}(h_\delta) = \sigma_{\mathrm{ac}}(h_\delta) = [0, \infty)$ for all values of the parameters R and Z, and that $\sigma_{\mathrm{sc}}(h_\delta) = \emptyset$. Moreover, there at most two eigenvalues in $\sigma_{\mathrm{d}}(h) \subset (-\infty, 0)$.

If $\sigma_{\mathrm{d}}(h) \neq \emptyset$, then the lowest energy $e_0 = \min\{\sigma_{\mathrm{d}}(h)\}$ is nondegenerate and its associated eigenvector ψ_0 can be chosen strictly positive, $\psi_0(x) > 0$ for all $x \in \mathbb{R}$.

4.4 Review of literature

A short review of literature follows. In section 4.4.1, articles focused on behavior of matter in strong magnetic fields, and working in a similar way as [BBjpa] and [BBfbs] are mentioned. In section 4.4.2, few papers concerning H_2^+ molecule are discussed more in detail, and a summary of original results of [BBjpa] and [BBfbs] is given.

4.4.1 Literature on strong magnetic fields

From the extensive literature concerning strong magnetic field several articles are shortly mentioned. We are interested primarily in those that use some approximative methods and asymptotic Hamiltonians, especially those with the singular potentials described by point interactions. As can be seen, these papers focus on the spectra of asymptotic Hamiltonians and their relation to the exact system, and investigate stability of matter and some basic properties such as equilibrium position and binding energy.

Reviews regarding strong magnetic fields can be found e.g. in [L2] and books [GHRW] and [SS].

Due to the impossibility to solve the exact system explicitly, the problem was treated in a number of alternative ways. The techniques used to investigate the system included variational approach, approximative methods involving the use of asymptotic Hamiltonians with miscellaneous effective and zero-range singular potentials, perturbation theory, finite elements method and numerical computations, and so forth.

The one-dimensional models with singular potentials have been used to study of the Coulomb problem for more than 50 years, c.f. [F]. These early papers mainly focused on simple atoms, but there were attempts to deal with more complex systems, an example being [LY]. As for the H_2^+ molecule, the δ-models appeared e.g. in [R2]. Therein, the existence of a stable groundstate was predicted for $Z > 0.374903$. In [BW], the H_2^+ molecule was investigated in a different manner: the Coulombic attractive potential was replaced with harmonic oscillator potentials while the repulsion term remained unchanged.

The first rigorous treatment of the atomic case appeared in [LSY1] (together with its twin [LSY2]) and [BSY].

In the paper [LSY1], the framework of the density functionals is used. The hyper-strong limit is considered $Z, B/Z^3 \to \infty$, and it is assumed that N/Z is uniformly bounded. Then it is proved the ground state of the exact system can be approximated by the Hartree mean-field model associated to the δ-model.

The paper [BSY] uses a variational approach to the exact Hamiltonian. The convergence of the ground state energy of H to that of h_δ is proven on $L^2(\mathbb{R}^N)$, using variational arguments; the angular momentum $\mathbb{M}$ is not fixed during the process.

In both papers, the ground state energy of H is rescaled first; that allows the comparison with that of h_δ for a fixed B. The variational approach used does not guarantee the existence of the ground state, and does not provide the information on its structure.

In some sense, stronger results were derived using the method of [BD3] described in detail in Section 4.2. This regards mainly the localization of the eigenvalues of H as discussed in Section 4.2.5.

The core of the method appeared already in [BD1] and [BD2], and the most advanced and most general description was summarized in [BD3]. In the first paper, an atomic ion with N bosonic electrons was studied, and the first two asymptotic operators h_{eff} and h_δ were introduced. In the second article, the spin and investigation of fermionic case was added. In the last paper, the third effective operator h_C appeared, and detailed study of the whole process was accomplished. It contains the strongest forms of the convergence theorems, too.

This method, with some modification, can be applied to some different systems as well. In [BBjpa] and [BBfbs], the H_2^+ molecule is studied by its means; the results will be mentioned in Section 4.4.2. Notice in particular that approximation of the ground state energy of the exact Hamiltonian using the δ-model includes explicit error bound, a property gained using the conclusions of Section 4.2.5.

As an example of other systems where this approach can be used, let us mention the two-dimensional electronic systems on a cylinder which describe excitons in carbon nanotubes, see [CDR].

The question under which conditions the state with the lowest energy occurs was discussed already in [AHS1] and [BS]. According to them, the ground state is reached for the positive values of angular momentum. Moreover, it was shown by variational computations that the lowest energies of the ground state are always attained for the parallel orientation of magnetic and inter-nuclei axes, see e.g. [TV]. Taken that into account, the ground state

has been proved to occur in the angular momentum $m = 0$ sector in [AH1].

The point interaction operators are used to model linear chains on n nuclei as well. With their use, the stability can be predicted and approximative values of ground state energies for H_3^{2+} and H_4^{3+} was found (c.f. [AMS]).

In [FLM], the Coulomb operator h_C for H_2^+ molecule was investigated.

4.4.2 Literature on H_2^+ molecule

In this section, a few articles concerning H_2^+ molecule will be discussed more in detail. Most importantly, a short review of results of [BBjpa] and [BBfbs] will be given. We will mention the results of one of their direct predecessors [BBDPO] as well. Finally, a new paper [H3] will gain our attention since some of its results confirm some of those obtained in [BBjpa] and [BBfbs].

Throughout this section, we will sometimes need to express explicitly the dependence of the energy e on Z, B, L or R. We will do it by writing e.g. $e[R, L, Z]$ without further notice.

Benguria, Brummelhuis et al., 2004

In [BBDPO], the equilibrium distance and binding energy are numerically investigated using a perturbative theory. Also the method formalized later in [BD3] is used.

Not taking the repulsion energy into consideration, the equivalent of the effective Hamiltonian h_{eff} defined in Section 4.2 is derived in the form

$$h_s^L = -\frac{\Delta_z}{2} - \frac{1}{L^2} V_L \tag{4.20}$$

with $V_L = V_L^+ + V_L^-$ and

$$V_L^{\pm} = \int_0^{\infty} \frac{e^{-u}}{\left(\frac{1}{L^2}\left(z \mp \frac{RL}{2}\right) + \frac{2u}{B}\right)} \, \mathrm{d}u.$$

Here $L = 2W(\sqrt{B}/2)$, see Section 4.1.3. The δ-Hamiltonian in established as

$$h_\delta = -\frac{1}{2}\Delta_z - \delta\left(z + a\right) - \delta\left(z - a\right)$$

where $a = RL/2$.

Then the perturbation method is deployed. One subsequently denotes a_0 the ground state of h_δ, ψ_0 its corresponding eigenfunction, and

$$\Delta V = h_s^L - h_\delta = \delta(z + a) + \delta(z - a) - \frac{1}{L^2} V_L.$$

Then approximation of the ground state energy of h_L to the second order in perturbation theory is then given by

$$e_2 = e_0 + tr(P_0 \Delta V P_0) - tr(P_0 \Delta V \widehat{r}_\delta \Delta V P_0)$$

where P_0 is the projector over ψ_0 and $\widehat{r}_\delta$ is the reduced resolvent; $tr(A)$ denotes the trace of an operator A. After fully incorporating the scaling and repulsion energy, one can compute the energy of the molecule as

$$E_2 = E_2[B, R] = L^2 e_2 + \frac{1}{R}.$$

The value of R for which the energy E_2 is minimized corresponds to the equilibrium distance R_{eq} between the nuclei, the binding energy being defined as $E_{\text{eq}} = E_2[B, R_{\text{eq}}]$.

The values of R_{eq} and E_{eq} are computed numerically for a range of magnetic field intensities. A good agreement with the results obtained using variational techniques is reached, see [BBDPO] and references therein. One can compute the corresponding eigenfunctions explicitly, too.

Later on, the perturbative results concerning the stability bounds obtained in this paper were found very close to those produced later by accurate variational (c.f. [TV]) and finite elements computations (c.f. [AH2]), at least when the second order computations were used.

Benguria, Brummelhuis et al., 2006

This part contains an overview of the most important results of [BBjpa] and [BBfbs]. As original results, both articles will be reproduced in full in Section 4.5.

We consider the homonucleus system with equal charges $Z = Z_1 = Z_2$ of the nuclei, and we choose $-R_1 = R_2 = R/2$, so (4.17) changes to

$$H = \frac{1}{2}\left(\frac{1}{\imath}\nabla - \frac{1}{2}\mathbb{B} \wedge r\right)^2 + \sigma \cdot \mathbb{B} - \frac{Z}{\left|r - \frac{R}{2}z\right|} - \frac{Z}{\left|r + \frac{R}{2}z\right|} + \frac{Z^2}{R}. \qquad (4.21)$$

Let us start with the discussion about the applicability of the machinery described in Section 4.2, and thus in turn about a possible approximation of the exact Hamiltonian (4.21) by the asymptotic operators. In a general setup with an arbitrary position of the nuclei, one could not use this approach since the total angular momentum $\mathbb{L}_z$ in the field direction is not preserved. However, $\mathbb{L}_z$ is a constant of motion in our special case due to the choice of parallel internuclear and magnetic field axes, and the employment of the method remains feasible.

We can thus establish the effective Hamiltonian in the form (4.20) as defined in [BBDPO]. However, we are primarily interested in the δ-Hamiltonian

$$h_\delta = -\frac{1}{2}\frac{d^2}{dx^2} - ZL\delta\left(z+\frac{R}{2}\right) ZL\delta\left(z-\frac{R}{2}\right) + \frac{Z^2}{R};$$

here $L = 2W(\sqrt{B}/2)$ which differs slightly from the definition in Section 4.1.3.

Moreover, the applicability of the method allows to derive a theorem similar to Theorem 1.5 of [BD3]. Here, the proof has to be modified due to different numbers of electrons and nuclei, leading i.a. to other values of the constants. However the structure of the molecular convergence theorem is the same as for the atomic case.

Theorem 1. *If d_δ is the distance of $\xi \in \mathbb{R}$ to the spectrum of h_δ, then there exist positive constants c_δ, C_δ and B_δ, only depending on Z, such that if $B \geq B_\delta$ and $c_\delta L \leq d_\delta \leq L^2/4$, then ξ is in the resolvent set of H, and*

$$||(H-\xi)^{-1} - (H_\delta - \xi)^{-1}|| \leq C_\delta \, \frac{L}{d_\delta^2}.$$

Using the explicit solvability of the δ-model, two eigenvalues of h_δ are explicitly found. Based on the analysis of the condition $\inf_R\{e_0 - e_\infty\} < 0$, with e_0 being the ground state energy and $e_\infty = \lim_{R\to\infty} e[R, L, Z]$ the energy in the separated atoms limit, the following stability theorem is derived.

Theorem 2. *The energy curve $e_0[R, L, Z] - e_\infty$ has:*
(i) a global strictly negative minimum if $Z/L \leq 0.3205$;
(ii) has a local minimum (corresponding to a resonance of the molecule) if $0.3205 < Z/L < 0.4398$ *and*
(iii) does not have a local minimum if $Z/L > 0.4398$.

The asymptotic behavior of the equilibrium r_e and the corresponding molecule energy $e_\mathrm{e} = e[r_\mathrm{e}, L, Z]$ are given by

$$\begin{aligned} r_\mathrm{eq} =& \frac{1}{2L^{3/2}\,Z^{1/2}}\left(1+\frac{5}{4}\theta+\frac{45}{32}\theta^2+O(\theta^3)\right), \\ e_\mathrm{min} =& -2Z^2L^2\left(1-2\theta+\frac{5}{4}\theta^2+O(\theta^3)\right), \end{aligned}$$

giving a starting position for the perturbative computations described in [BBDPO]. A prediction of existence of He_2^{3+} is made as well.

Finally, the the arguments of Section 9 of [BD3] (and summarized here in Section 4.2.5), are used to conclude that the ground state energy E_0 of the exact Hamiltonian H can be estimated by its δ-counterpart, namely

$$|E_0 - e_0| \leq c_\delta L,$$

this bound being uniform in R. The technical difficulties caused by the second eigenvalue e_1 of h_δ, blocking the fulfillment of the assumptions in Theorem 1.5 of [BD3], are avoided by deploying the symmetry argument. Thus, it is proved that the equilibrium distance $R_{\rm e}$ of the exact system lies between the two roots of the equation

$$e_{\min} + c_\delta L = e[R, L, Z] - c_\delta L.$$

That leads to this last theorem.

Theorem 3. *For sufficiently large B, ground state energy and equilibrium distance of the H_2^+-molecule (4.21) is given by, respectively*

$$E_0[L, Z] = -2L^2Z^2 + 4Z^{5/2}L^{3/2} + \mathcal{O}(L),$$

and

$$R_{\rm eq} = \frac{1}{2L^{3/2}\,Z^{1/2}} + \mathcal{O}\left(L^{-7/4}\right).$$

The convergence of H_2^+ to its united atom limit He^+ is then discussed, and it can formally be described as

$$\frac{E_0^{H_2^+}(B)}{E_0^{He^+}(B)} \to 1, \quad B \to \infty.$$

However, two caveats are mentioned, being the relativistic effect and inaccuracy caused by the infinity nuclei mass approximation.

Hogreve, 2009

In 2009, a new analysis of the H_2^+ system appeared in [H3]. Therein, the system is described by the Hamiltonians

$$h = -\frac{1}{2}\frac{d^2}{dx^2} - Z_1\delta_{R_1} - Z_2\delta_{R_2}$$

and

$$H = h + \frac{Z_1Z_2}{R}.$$

Based on properties of the corresponding quadratic form, analytic dependence of eigenvalues and eigenvectors on Z and R is proven. Based on that, the following analogy of the molecular virial theorem is established: If $R > 0$ and $e \in \sigma_{\rm d}(h)$, then

$$\frac{de}{dR} = -2R^{-1}e + R^{-1}\langle V\rangle$$

where $\langle V\rangle = -\sum_{i=1}^{2}\langle\psi, Z_i\delta_{R_i}\psi\rangle$. For equilibria $R_{\rm e}$ of H, and for corresponding energy $e_{\rm e} = e[R_{\rm e}, Z]$ and eigenstate $\psi_{\rm e}$ that implies

$$-R_{\rm e}\sum_{i=1}^{2} Z_i\,|\psi_{\rm e}(R_i)|^2 = 2e_{\rm e} + \frac{Z_1Z_2}{R_{\rm e}}.$$

Then the electronic curves, i.e. the eigenvalues $e = e[R, Z]$ considered as functions of R and Z, are then studied. First, the united atom limit $R \downarrow 0$ is examined.

Theorem 4.1. *If $Z_1+Z_2 > 0$, then for $R \downarrow 0$ the ground state energy behaves as*

$$e_0 = -(Z_1 + Z_2)^2/2 + 2(Z_1 + Z_2)Z_1Z_2R + O(R^2).$$

If $Z_1 = -Z_2 = Z > 0$, then upon $R \downarrow 0$ the ground state energy hits the continuum in the united atoms limit with

$$e_0 = -2Z^4R^2 + O(R^3).$$

If the ground state or excited energy is absorbed into $\sigma_{\rm ess}(h)$ at $R_a = (Z_1^{-1} + Z_2^{-1})/2 > 0$, then the approach $R \downarrow R_a$ to the continuum is characterized by

$$e_0 = -2(Z_1^{-1} + Z_2^{-1})^{-2}(R - R_a)^2 + O((R - Ra)^3).$$

Then the bounds from below and above, corresponding to the united and separated atoms limits, respectively, are established.

Theorem 4.2. *If $Z_1, Z_2 > 0$, then all energies $e \in \sigma_{\rm d}(h)$ are bounded below by the ground state energy of the united atoms limit, i.e., for all $R \geq 0$*

$$e \geq e_0[0, Z] = -(Z1 + Z2)^2/2.$$

Upper bounds on the ground state energy are provided by the separated atoms limit energies, i.e., for all $R \geq 0$

$$e_0 < \min_{i=1,2} e_0[0, (Z_i, 0)] = -(\max\{Z_1, Z_2\})^2/2.$$

In the presence of a negative charge, $Z_1 > 0$, $Z_2 < 0$, the latter bound turns into a lower bound such that for all $R \geq 0$

$$e > e_0[0, (Z_1, 0)] = -Z_1^2/2.$$

This is then used to prove the final theorem that focuses on the monotony of the electronic curves.

Theorem 4.3. *If $Z_1, Z_2 > 0$, then the electronic ground state curve e_0 is strictly monotonously increasing in $R \geq 0$. In case that $-Z_1 \leq Z_2 < 0$, the ground state curve is strictly monotonously decreasing.*

As a final step, a stability analysis is preformed. It is showed that the behavior in this aspect is the same as compared to the exact system (4.18). Here, the key role plays the asymmetry characterized by the ratio Z_1/Z_2. With respect to that quantity, three potential modes can occur: stability, metastability with the dissociation possible due to tunneling, and instability where the potential barrier disappears. Taking fixed ratios $\eta = Z_2/Z_1$, the following results are stated.

Stability holds for $0 < Z_1^{(c)}(\eta)$ with

$$Z_1^{(c)}(\eta) = \sup\{Z_1 > 0 | E_\mathrm{e} < E_\infty\}.$$

Here $E_\mathrm{e} = E[R_\mathrm{e}, Z]$ is the energy at the equilibrium position (defined as the leftmost minimum of $e[R, Z]$ with respect to r, or $R_\mathrm{e} = \infty$ if there is no minimum), and $E_\infty = E[\infty, Z] = \lim_{R\to\infty} E[R, Z]$ is the separated atoms limit energy.

Then, metastable regime occurs for $Z_1^{(c)} < Z_1 < Z_1^{(m)}$ where

$$Z_1^{(m)} = \sup\{Z_1 > Z_1^{(c)}(\eta) | E_\mathrm{e} < \sup_{R\geq R_\mathrm{e}} E\}.$$

Both $Z_1^{(c)}$ and $Z_1^{(m)}$ are then derived. First, one has that

$$Z_1^{(c)}(\eta) = \max_{1\leq\alpha\leq 1+\eta} \{(4\pi\alpha)^{-1}(1-\alpha^2)\log((\alpha-1)(\eta^{-1}\alpha-1))\}$$

For homonuclear systems with $Z_1 = Z_2 = Z$ and $\eta = 1$ the following value is found,

$$Z^(c) = \max_{1\leq\alpha\leq 2} \{(2\alpha)^{-1}(1-\alpha^2)\log(\alpha-1) = 0.320483362463\ldots$$

agreeing exactly with the value found in [BBjpa] and [BBfbs].

The same holds true for $Z_1^{(m)}$ with the general formula

$$Z_1^{(m)} = \max_{1\leq\alpha\leq 1+\eta} \left\{ \frac{(\alpha-1)(\eta^{-1}\alpha-1)(\log(\alpha-1)(\eta^{-1}\alpha-1))}{2(2\alpha-1-\eta-\alpha^{-1}\eta(\alpha-1)(\eta^{-1}\alpha-1)\log(\alpha-1)(\eta^{-1}\alpha-1))} \right\}$$

and the special homonuclear value

$$Z^{(m)} = \max_{1\leq\alpha\leq 2}\left\{\frac{(\alpha-1)^2(\log(\alpha-1))^2}{\alpha-1-\alpha^{-1}(\alpha-1)^2\log(\alpha-1)}\right\} = 0.439841890466\ldots$$

confirming [BBjpa] and [BBfbs] again.

4.5 Original results

This section contains the original results as published in the articles [BBjpa] and [BBfbs]. They are stated in full, the former in Section 4.5.1, and the latter in Section 4.5.2.

4.5.1 Asymptotic behaviour of the equilibrium nuclear separation for the H_2^+ molecule in a strong magnetic field

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Asymptotic behaviour of the equilibrium nuclear separation for the H_2^+ molecule in a strong magnetic field

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Abstract We consider the hydrogen molecular ion H_2^+ in the fixed nuclear approximation, in the presence of a strong homogeneous magnetic field. We determine the leading asymptotic behaviour for the equilibrium distance between the nuclei of this molecule in the limit when the strength of the magnetic field goes to infinity.

1 Introduction

One dimensional Hamiltonians with delta function interactions have been used for a long time as toy models in atomic physics (see, e.g., [5], and references therein). However, with the study of matter in the presence of strong magnetic fields, these models have become more physically relevant.

It is now well established that atoms and molecules in the presence of a strong uniform magnetic field behave like systems in one dimension. In fact, a strong magnetic field confines the electrons to Landau orbitals which are orthogonal to the direction of the applied magnetic field. In this manner,

only the behaviour of the electrons along the direction of the magnetic field is subject to the influence of their Coulomb interaction with the nuclei, or to the interaction among themselves. Since one can extend the results of [4, section 9], to the present molecular case, this genuine molecular case reduces effectively to the one dimensional ion model where coulombic interactions between the electron and the nuclei are replaced by delta point interactions, see (1) below.

2 The asymptotic model

Our model consists of two nuclei, each one of nuclear charge Z, separated by a distance R. As we have discussed in the Introduction, for large values of the magnetic field, the molecule we are considering is described by an asymptotic model defined by the following Hamiltonian,

$$H = L^2 Z^2 \left[\frac{p_z^2}{2} - \delta\left(z - \frac{RLZ}{2}\right) - \delta\left(z - \frac{RLZ}{2}\right)\right] + \frac{Z^2}{R}, \qquad (1)$$

acting on $L^2(\mathbb{R})$ (see [1] for more details). The parameter L that appears in this Hamiltonian depends on the strength of the magnetic field and it is given explicitly by $L = 2W(\sqrt{B}/2)$, where W is the Lambert function [6]. If one considers the function $y(x) = x\exp(x)$, for $x \in [0, \infty)$, the Lambert function is its inverse, i.e., $x = W(y)$. It is elementary to derive the following asymptotics:

$$L = \log B - 2\log(\log B) + \mathcal{O}\left(\frac{\log(\log B)}{\log B}\right), \quad B \to \infty.$$

The ground state energy of this system, which is a function of R, Z, and L, can be computed in closed form in terms of the Lambert function, and it is given by

$$E(R, L, Z) = -L^2\, Z^2 \frac{\alpha_0^2}{2} + \frac{Z^2}{R}, \qquad (2)$$

where

$$\alpha_0 \equiv 1 + \frac{W(R\,L\,Z e^{-RLZ})}{RLZ}.$$

The first term in (2) is the electronic energy, while the second term is just the Coulomb repulsion between the nuclei.

In this section we study the dependence of the ground state energy E, of the asymptotic model, on the nuclear separation R. In particular, we shall determine for which values of the parameters Z and L, the asymptotic model exhibits binding.

Let

$$F(x) \equiv \frac{1}{2}\left(x + W(xe^{-x})\right)^2 . \tag{3}$$

In terms of $F(x)$, the ground state energy of H can be written as

$$E(R, L, Z) = -\frac{F(R\,L\,Z)}{R^2} + \frac{Z^2}{R} = \frac{L^2\,Z^2}{x}\left(\frac{Z}{L} - \frac{F(x)}{x}\right), \tag{4}$$

where $x = R\,L\,Z$. When the nuclei are infinitely apart, the ground state energy of H is given by

$$E_{\rm at} = -\frac{Z^2 L^2}{2}. \tag{5}$$

As usual, we define the *binding energy* of the molecule as the difference

$$E_B = \sup_R \left[E_{\rm at} - E(R, L, Z)\right]. \tag{6}$$

The molecule will exist (in the frame of this asymptotic model) if and only if $E_B > 0$, i.e., if $E_{\rm at} - E(R, L, Z) > 0$ for some $R \in (0, \infty)$. In case $E_B > 0$, we will denote $R_{\rm eq}$ the value of R which maximizes $E_{\rm at} - E(R, L, Z)$. $R_{\rm eq}$ is the actual separation between the nuclei of the molecule described by the asymptotic model.

In terms of $x = R\,L\,Z$ and the Lambert function, we can write

$$E_{\rm at} - E(R, L, Z) = \frac{L^2\,Z^2}{x}\left(J(x) - \frac{Z}{L}\right), \tag{7}$$

where

$$J(x) \equiv \frac{F(x)}{x} - \frac{x}{2} = \frac{(2x + W(xe^{-x}))W(xe^{-x})}{2x}. \tag{8}$$

Using (7), we see that there will be a molecule in the asymptotic model provided there is an x for which $J(x) > Z/L$. One can readily check that the function $J(x)$ is positive in $(0, \infty)$, $J(0) = 0$ and $\lim_{x\to\infty} J(x) = 0$. Moreover, $J(x)$ has only one maximum in $(0, \infty)$, located at $x_J \approx 0.84$, and $J(x_J) \approx 0.3205$, see lemma 1 in Appendix. Thus, if $(Z/L) < J(x_J)$, the molecule exists (in other words, there is a global minimum of $-E_{\rm at} + E(R, L, Z)$, and therefore $E_B > 0$.

In case $Z/L > J(x_J)$, the molecule will not bind. However, there could still be a local minimum of $-E_{\rm at} + E(R, L, Z)$ in $(0, \infty)$. If there is a local minimum, but $E_B \leq 0$, we will say that there is a *resonance*. To study local minima, we compute

$$\frac{\partial E}{\partial R}(R, L, Z). \tag{9}$$

Using (4) and the properties of the Lambert function we can express,

$$\frac{\partial E}{\partial R}(R, L, Z) = \frac{LZ}{R^2}\left(G(x) - \frac{Z}{L}\right), \tag{10}$$

where, as before, $x = R\,L\,Z$, and

$$G(x) \equiv \frac{(x + W(xe^{-x}))^2 W(xe^{-x})}{x(1 + W(xe^{-x})}. \tag{11}$$

Using the properties of the Lambert function, one can check that the function $G(x)$ is positive in $(0, \infty)$, $G(0) = 0$, $\lim_{x\to\infty} G(x) = 0$. Moreover, $G(x)$ has a unique maximum in this interval, attained at $x_G \approx 1.95$, and $G(x_G) \approx 0.4398$, see lemma 2 in Appendix. One can compare the functions J and G defined above. It turns out that $J(x) \geq G(x)$ if $0 \leq x \leq x_J$, whereas $J(x) \leq G(x)$, if $x_J \leq x < \infty$, hence $G(x_J) = J(x_J)$ (i.e., both functions agree at the maximum of J). From (10) and the properties of G we see that if $Z/L > G(x_G)$, $-E_{\rm at} + E(R, L, Z)$ does not have a local minimum in $(0, \infty)$. On the other hand, if $J(x_J) < Z/L < G(x_G)$, $-E_{\rm at} + E(R, L, Z)$ has a local minimum, i.e., we will have a *resonance*.

We can summarize our discussion above in the following theorem. See also Figure 1 below.

Theorem 1. *For the system described by the Hamiltonian (1), the energy curve $-E_{\rm at} + E(R, L, Z)$,*
a) has no local minimum if $G(x_G) \approx 0.44 < \frac{Z}{L}$,
b) has a local minimum if $J(x_J) \approx 0.32 < \frac{Z}{L} < G(x_G) \approx 0.44$.
c) has a global minimum (i.e, there is binding) if $\frac{Z}{L} < J(x_J) \approx 0.32$. We denote by R_{eq} the position of this minimum.

For fixed nuclear charge Z, Z/L can be made arbitrarily small by choosing the strength of the magnetic field sufficiently large, since $L = 2W(\sqrt{B}/2)$. Hence, for sufficiently large B, $-E_{\rm at} + E(R, L, Z)$ will have a global minimum. In this case, it follows from (10) that the position of this minimum is given by

$$R_{\rm eq} = \frac{1}{L\,Z} G^{-1}(\frac{Z}{L}). \tag{12}$$

If $Z/L \ll 1$, we get from (12) and (A.20) in the Appendix that

$$R_{\rm eq} = \frac{1}{2}\frac{1}{L^{3/2}\,Z^{1/2}} + \frac{5}{8}\frac{1}{L^2} + \frac{45}{64}\frac{Z^{1/2}}{L^{5/2}} + \frac{1}{L^2} O\left(\frac{Z}{L}\right). \tag{13}$$

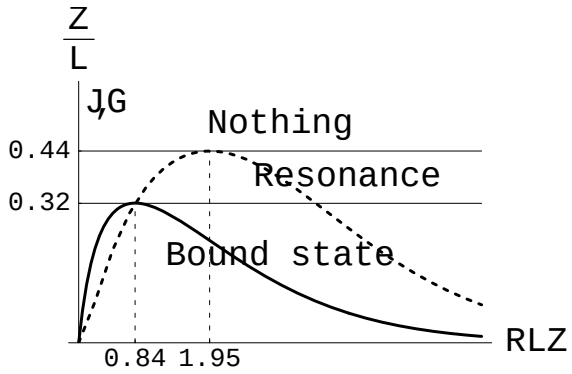

Figure 4.1: Graphs of J (thick solid curve), G (thick dashed curve). and Z/L (thin horizontal lines)

For $Z/L \ll 1$, the minimum value of the energy, $E(R_{\rm eq}, L, Z)$ can be obtained, to leading order, using (4), (13), and (A.17) in the Appendix. Thus we obtain,

$$E_{\rm min} \equiv E(R_{\rm eq}, L, Z) = -2Z^2L^2\left(1 - 2\theta + \frac{5}{4}\theta^2 + O(\theta^3)\right), \qquad (14)$$

where we have set $\theta = \sqrt{Z/L}$.

For our discussion below, it is convenient to give the asymptotic behaviour of the whole energy curve, $E(R, L, Z)$, for large values of the magnetic field (i.e., for large values of L). Using (4) and the asymptotic properties of $F(x)$, given in the Appendix, see (A.17), we obtain

$$E(R, L, Z) = \frac{L^2Z^2}{x}\left(\frac{Z}{L} - 2x + 4x^2 - 10x^3 + O(x^4)\right) \qquad (15)$$

with $x = RLZ$. This asymptotic behaviour is valid for values of R such that $R \ll \frac{1}{LZ}$.

3 The leading behaviour of the nuclear separation of the H_2^+ molecule in the presence of a strong magnetic field

With the help of the calculations on the asymptotic model of Section 2, we will compute the leading behaviour of the equilibrium nuclear separation of the H_2^+ molecule, in the limit when the strength of the magnetic field goes to infinity. Since we are interested in the H_2^+ molecule, we set $Z = 1$ throughout

this section. Denote by $r_{\rm eq}$ the equilibrium distance between the nuclei of the H_2^+ molecule in the presence of a strong magnetic field. Here we will prove the following estimate for $r_{\rm eq}$.

Theorem 2.

$$r_{\rm eq} = \frac{1}{2L^{3/2}} + \mathcal{O}(L^{-\frac{7}{4}}), \quad \textit{as } B \to \infty \tag{16}$$

where $L = 2W(\sqrt{B}/2)$ *and* W *is the Lambert function (*[6]*).*

In [4], we have said that the ground state energy of the H_2^+ molecule can be estimated in terms of the ground state energy of the asymptotic model, using the norm–resolvent convergence method developed by Brummelhuis and Duclos in [4]. We will denote by $E(R, L, 1)$ the ground state energy of the aymptotic model studied in Section 2, for $Z = 1$ and by $e(R, L, 1)$ the ground state energy of the asymptotic model. As said in [1], for B large enough one has,

$$E(R, L, 1) - \alpha_- \leq e(R, L, 1) \leq E(R, L, 1) + \alpha_+, \tag{17}$$

where $\alpha_\pm$ are positive constants that only depend on L. Moreover,

$$\alpha_+ + \alpha_- = c\, L \tag{18}$$

where c is a constant, independent of L and R. These two above equations can be derived with the method of [4], see in particular Theorem 1.5 and section 9, there.

In section 2, we have computed the equlibrium distance, $R_{\rm eq}$ (13), and the minimum energy, $E_{\rm min}$, (14) for the asymptotic delta–model. Given these values and the error estimates embodied in (17) and (18) above, we can estimate the actual separation of the nuclei of the H_2^+ molecule in the presence of a strong magnetic field. In the figure, we have pictured the energy curve for the asymptotic model, $E(R, L, 1)$, as well as the curves $E(R, L, 1) \pm \alpha_\pm$. Recall that we denote by $r_{\rm eq}$ the equilibrium distance of the nuclei of the real molecule in the presence of a strong magnetic field; it follows from the figure that

$$R_1 < r_{\rm eq} < R_2 \tag{19}$$

where R_1 and R_2 are the solutions of the equation

$$E_{\rm min} + \alpha_+ = E(R, L, 1) - \alpha_-$$

i.e.,

$$E_{\rm min} + cL = E(R, L, 1); \tag{20}$$

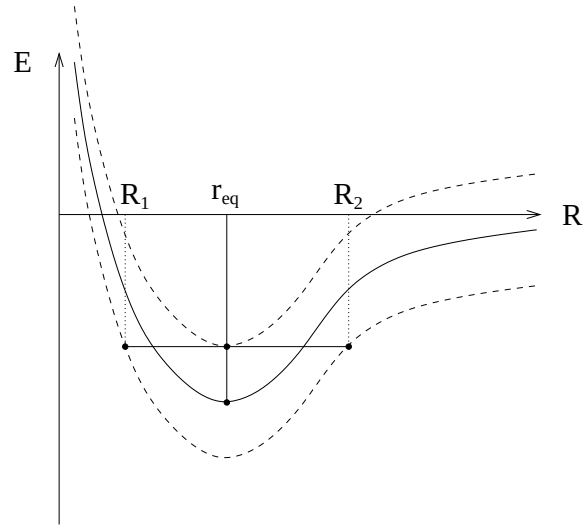

Figure 4.1: A sketch of the curves $R \to E(R, L, Z)$ and $R \to E(R, L, Z) \pm \alpha_{\pm}$ with the points $R_{1,2}$ and r_{eq}

one can see easily that they both go to 0 as $L \to \infty$, see the end of Appendix. Replacing the asymptotic behaviour (14) for $E_{\min}$ (with $Z = 1$), and (15) for $E(R_i, L, 1)$ in (20), we get

$$\begin{aligned} -2L^2 \left(1 - 2L^{-1/2} + \frac{5}{4}L^{-1} + O(L^{-3/2})\right) + cL = \\ = \frac{L^2}{x}\left(\frac{1}{L} - 2x + 4x^2 - 10x^3 + O(x^4)\right), \end{aligned} \tag{21}$$

where $x = R_i L$ (since $Z = 1$). It follows that

$$(1 - 2L^{\frac{1}{2}}x)^2 = (c - \frac{5}{2})x + 10x^3 L + \mathcal{O}(x^4 L) + \mathcal{O}(L^{-\frac{1}{2}}x). \tag{22}$$

Assume now that $L^{\frac{1}{2}}x$ is not bounded, this would mean that there exists a subsequence of L values so that $L^{\frac{1}{2}}x \to \infty$. Substituting this sequence in (22) gives:

$$4Lx^2 \sim (c - \frac{5}{2})x + 10x^3 L \sim 10x^3 L$$

since $x^2 L \to \infty$; however this is a contradiction. Using in (22) that $R_i L^{\frac{3}{2}} = xL^{\frac{1}{2}}$ is bounded gives

$$R_i = \frac{1}{2L^{\frac{3}{2}}} + \mathcal{O}(L^{-\frac{7}{4}}).$$

which proves the theorem.

Appendix

Definition 1. *We define the function $J(x)$ as*

$$J(x) \equiv W(y) + \frac{W(y)^2}{2x}, \tag{A.1}$$

for all $0 \leq x < \infty$, where $y = x\exp(-x)$, and W denotes the Lambert function, i.e., the nonnegative solution of $W(x)\exp(W(x)) = x$. Since in the sequel W as well as its derivative is always evaluated at $y = x\exp(-x)$, we shall sometimes omit this argument.

In our next lemma, we prove some properties of $J(x)$ needed in the main body of the manuscript.

Lemma 1. *The function $J(x)$ is positive in $(0, \infty)$, it is real analytic, it has a unique maximum, with value $\max J \sim 0.32$ taken at $x_J \sim 0.84$.*

Proof. That J is positive in $(0, \infty)$ follows immediately from (A.15) and the definition of W. The Lambert function is real analytic. Moreover, for small values of its argument, $W(y) = y + \mathcal{O}(y)$, thus $W(y)^2/2x$ will be also real analytic in $(0, \infty)$. Hence, we need only prove that J has a unique critical point (a maximum) in $(0, \infty)$. Taking the derivative of (A.15) with respect to x, we get,

$$\frac{dJ}{dx} = \frac{dW}{dy}\frac{dy}{dx} + W\frac{dW}{dy}\frac{dy}{dx}\frac{1}{x} - \frac{W(y)^2}{2\,x^2}. \tag{A.2}$$

From the definition of the Lambert function, it follows that

$$\frac{dW}{dy} = \frac{W(y)}{y(1+W(y))}, \tag{A.3}$$

and from the definition of $y = x\exp(-x)$ we have

$$\frac{dy}{dx} = \frac{y}{x}(1-x). \tag{A.4}$$

Using (A.16), (A.3), and (A.18) we get,

$$\frac{dJ}{dx} = \frac{W(y)}{2(1+W(y))x^2}j(x), \tag{A.5}$$

where we have set

$$j(x) = 2x(1-x) + 2W(y)(1-x) - W(y)(1+W(y)). \tag{A.6}$$

Since W is positive in $(0,\infty)$, the sign of $j(x)$ determines the sign of dJ/dx. The function $j(x)$ is clearly negative for $x > 1$. On the other hand, we can rewrite,

$$j(x) = x(1-2x) + x(1-2W(y)) + W(y)(1-W(y)). \tag{A.7}$$

Since $W(y) \leq y$, and $y = xe^{-x} < x \leq 1/2$, if $0 \leq x \leq 1/2$, it follows from (A.7) that $j(x) > 0$ for all $x \in (0, 1/2)$. Using (A.3) and (A.18), we can compute,

$$x(1+W(y))j'(x) = x(1+W)[2(1-2x)-2W]+(1-x)W\,[(1-2x)-2W]. \tag{A.8}$$

In the interval $(1/2, 1)$ each of the terms on the right side of (A.8) is negative. Hence, $j(x)$ is decreasing in $(1/2, 1)$. In summary, $j(x) > 0$ in $(0, 1/2)$, $j(x)$ is strictly decreasing in $(1/2, 1)$and $j(x) < 0$ in $(1, \infty)$. From here it follows that $j(x)$ has a unique zero in $(0, \infty)$. If we denote x_J this zero, it follows from the proof that $1/2 < x_J < 1$. Numerically, $x_J \approx 0,84$. □

Definition 2. *We define the function $G(x)$ as*

$$G(x) \equiv \frac{W(y)(x+W(y))^2}{x(1+W(y))}, \tag{A.9}$$

for all $0 \leq x < \infty$ where, as before, $y = x\exp(-x)$, and W denotes the Lambert function. Concerning the function $G(x)$, in our next lemma, we prove some properties needed in the main body of the manuscript.

Lemma 2. *The function $G(x)$ is positive in $(0,\infty)$, it is real analytic, it has a unique maximum $\max G \sim 0.44$ taken at $x_G \sim 1.95$. Moreover, the functions $J(x)$ and $G(x)$ intersect at a unique point in $(0,\infty)$ precisely at $x = x_J$.*

Proof. Let's begin by proving that G and J only cross at x_J, i.e., at the maximum point of $J(x)$. From (A.15) and (A.9), we see that the equation $G(x) = J(x)$ can be simplified to read,

$$2x - 2x^2 - 2xW = W^2 - W.$$

which is precisely the condition $j(x) = 0$ (see equation (A.7) above), which has only one solution which we have denoted by x_J. □

Now, using (A.9), (A.3) and (A.18), after some simplifications we can write,

$$\frac{dG}{dx} = \frac{(W+x)W}{x^2(1+W)^2}g(x), \tag{A.10}$$

where we have set

$$g(x) \equiv 2W(y)(1-x) + (x - W(y))(1 + W(y)) + \frac{1}{1+W(y)}(W + x)(1 - x). \tag{A.11}$$

If $x < 1$, the first and the last term of (A.11) are positive. On the other hand, $y < x$ and $W(y) < y$ imply that the second term is also positive. Thus, $g(x) > 0$ if $0 < x < 1$. Moreover, we can regroup terms in (A.11) to write

$$(1 + W(y))g(x) = (2 - x)(W(y) + x) - xW(y)^2 - W(y)^3. \tag{A.12}$$

From (A.12) it follows that $g(x) < 0$ if $x > 2$. Finally, we can compute

$$\phi(x) \equiv x(1 + W(y))[(1 + W)g]', \tag{A.13}$$

using as before (A.3) and (A.18). After several simplifications, we get,

$$\phi(x) = 2W(1 - x) + 2xW^2(x - 2) + 2(1 - x)x + 2W^3(x - 2) - (x^2 - W^2)W. \tag{A.14}$$

If $1 < x < 2$, the first four terms of (A.14) are negative. The last term is also negative, since $W < x$. In summary, $(1 + W)g(x) > 0$ in $(0, 1)$, $(1 + W)g(x)$ is strictly decreasing in $(1, 2)$and $(1 + W)g(x) < 0$ in $(2, \infty)$. From here it follows that $g(x)$ has a unique zero in $(0, \infty)$. If we denote x_G this zero, it follows from the proof that $1 < x_G < 2$. Numerically, $x_G \approx 1, 95$.

We continue this appendix by giving the leading behaviour of several special functions that are used in this manuscript. We begin with the leading behaviour of the Lambert function. From the definition of W we have,

$$W(x) = x - x^2 + \frac{3}{2}x^3 - \frac{8}{3}x^4 + O(x^5). \tag{A.15}$$

In fact, $W(x) = \sum_{n=1}^{\infty} x^n(-n)^{n-1}/n!$. From (A.15) it follows that

$$W(xe^{-x}) = x - 2x^2 + 4x^3 - \frac{28}{3}x^4 + O(x^5). \tag{A.16}$$

For the function $F(x)$, defined by (3) we have

$$F(x) = 2x^2\left[1 - 2x + 5x^2 + O(x^3)\right]. \tag{A.17}$$

Hence, for $J(x)$ defined by (8) we obtain,

$$J(x) = \frac{3}{2}x - 4x^2 + 10x^3 + O(x^4). \tag{A.18}$$

whereas for the function $G(x)$, defined by (11) we get

$$G(x) = 4x^2 \left[1 - 5x + 20x^2 + O(x^3)\right]. \tag{A.19}$$

From (A.19) we obtain the leading behaviour of $G^{-1}(x)$, which is given by

$$G^{-1}(x) = \frac{1}{2}x^{1/2} + \frac{5}{8}x + \frac{45}{64}x^{3/2} + O(x^{5/2}). \tag{A.20}$$

We end up this appendix by proving that both roots R_1 and R_2 of the equation $E_{\min} + \alpha_+ = E(R, L, 1) - \alpha_-$ tends to 0 as $L \to \infty$, see the proof of theorem 2. This is clear for R_1 since it bounded by $R_{\rm eq}$. Then one has thanks to (14)

$$E(R_2, L, 1) = cL + E_{\min} \sim -2L^2. \tag{A.21}$$

Assume first that $R_2 L$ is bounded below at least for a subsequence of values L which tends to ∞. Then on this subsequence one has

$$E(R_2, L, 1) \sim -L^2 \frac{F(R_2 L)}{(R_2 L)^2}$$

since $F(x)/x$ is bounded below by a positive constant on $[x_0, \infty[$, $x_0 > 0$. Using that $F(x)/x^2 < 2$ on all intervals $[x_0, \infty[$, $x_0 > 0$ this contradict (A.21). Thus one has $R_2 L \to 0$ as $L \to \infty$.

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4.5.2 Non-relativistic H_2^+ molecule in a strong magnetic field

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Non-relativistic H_2^+-molecule in a strong magnetic field

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Abstract We show that under the influence of a strong uniform magnetic field the energy of the H_2^+-ion at the 0-th order Born-Oppenheimer approximation goes over into that of the corresponding united atom limit, He^+.

1 Introduction

Atoms and molecules in a strong uniform magnetic field of strength B will effectively behave like systems in one dimension, since the field will 'freeze' the motion of the electrons perpendicular to the field into Landau orbitals. The electrons will only be free to move along the field-direction, under the influence of one-dimensional effective potentials induced by the original Coulomb interactions. In the high field limit, these effective potentials are well-approximated by zero-range δ-interactions, with a B-dependent coupling constant. This physical picture can be given a rigorous mathematical foundation for atoms and molecules having infinitely heavy nuclei aligned along the field direction, with the successive approximations holding true in the fairly strong sense of norm-convergence of resolvents, and explicit error bounds ([1, 2, 4, 3, 5]).This can be used to draw rigorous conclusions, for the original atomic or molecular Hamiltonian, from the δ-model, which in one-electron cases is elementary solvable. We illustrate this by a detailed study

of the H_2^+-molecule in a strong magnetic field, for which we prove that the equilibrium distance between the nuclei tends to 0 as the field strength tends to infinity, and the ground state energy tends to that of its united atom limit.

2 The Asymptotic Model

We consider a non-relativistic one-electron homonuclear diatomic molecule with fixed nuclei of charge Z in a strong homogeneous magnetic field $\mathbb{B} = B\hat{z}$, where $\hat{z}$ is the unit vector in the z-direction. If the inter-nuclear distance is R, then the Pauli-Hamiltonian for the molecule, in atomic units, is:

$$H = \frac{1}{2}\left|p - \frac{1}{2}r \wedge \mathbb{B}\right|^2 + \sigma \cdot \mathbb{B} - V + \frac{Z^2}{R}, \tag{1}$$

where V is the electron-nuclei potential:

$$V(r) = \frac{Z}{|r - \frac{R}{2}\hat{z}|} + \frac{Z}{|r + \frac{R}{2}\hat{z}|}, \tag{2}$$

and $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ the electron spin vector, given by the Pauli matrices. The conversion to the field strength in Gauss is done by multiplication of B by $B_0 := m_e^2 e^3 c/\hbar^3 =\simeq 2.35\ 10^9$ G. In [5], it was shown that atomic Hamiltonians in strong magnetic fields can be approximated, in norm-resolvent sense, by a hierarchy of *effective Hamiltonians* describing one-dimensional atoms on the line. The machinery of [5] is still applicable to the molecular case, provided the nuclear axes are taken parallel to $\mathbb{B}$, to ensure that total electron-angular momentum in the field direction is preserved (this is no longer true for arbitrary orientations). The simplest of the effective Hamiltonians of [5], [4], giving the lowest order approximation, is the δ-Hamiltonian, which in the present case is given by

$$h_\delta = \frac{1}{2}p_z^2 - \sum_{\pm} ZL\delta\left(z \pm \frac{R}{2}\right) + \frac{Z^2}{R}. \tag{3}$$

Here $L = L(B) := 2W(\sqrt{B}/2)$, $W : [-e^{-1}, \infty) \to \mathbb{R}$ being the principal branch of the *Lambert function*, defined as the unique real solution of $W(x)e^{W(x)} = 1$ which is positive for positive x; see e.g. [6]. Note that h_δ still depends on B, through L. We have that $L(B) \simeq \log B$ as $B \to \infty$.

Under the reasonable assumption that the electron is in an s-state (this is not essential), h_δ will approximate H in the following sense: let Π_0 be the orthogonal projection onto the lowest Landau band of the 'free' operator $\frac{1}{2}|p - \frac{1}{2}r \wedge \mathbb{B}|^2)$ with $m = 0$, and let $\Pi_0^\perp$ be the projection onto the orthogonal complement; Π_0 commutes with H, and h_δ has a natural interpretation as an operator on $\mathrm{Ran}(\Pi_0)$. Let $H_\delta := h_\delta\Pi_0 + H(B)\Pi_0^\perp$. Then:

Theorem 1. *(compare* [5]*, thm. 1.5) If $d_\delta(\xi)$ is the distance of $\xi \in \mathbb{R}$ to the spectrum of h_δ, then there exist positive constants c_δ, C_δ and B_δ, only depending on Z, such that if $B \geq B_\delta$ and $c_\delta L \leq d_\delta(\xi) \leq L^2/4$, then ξ is in the resolvent set of H, and*

$$||(H-\xi)^{-1} - (H_\delta - \xi)^{-1}|| \leq C_\delta \, \frac{L}{d_\delta(\xi)^2}. \tag{4}$$

The spectrum of $H\Pi_0^\perp$ turns out to be positive, and $d_\delta(\xi) > 0$ will imply that $\xi < 0$, since the essential spectrum of h_δ already contains $[0, \infty)$. Theorem 1 allows us to deduce information about the negative bound states of H from those of h_δ. Equation (4) may look strange as an approximation result, since the L in the left hand side goes to ∞. However, the ground state energy of h_δ is of the order of $-cL^2$ in absolute value, and the same can then be shown to be the case for H, see below. In [1]-[3], as re-scaled version of theorem 1 was used.

The δ-model is explicitly solvable, and h_δ can be shown to have two eigenvalues,

$$\begin{aligned} e_0 = e_0(R,L,Z) &= -\frac{1}{2}(LZ)^2 \left(1 + \frac{W\left(xe^{-x}\right)}{x}\right)^2 + \frac{Z^2}{R}, \\ e_1 = e_1(R,L,Z) &= -\frac{1}{2}(LZ)^2 \left(1 + \frac{W(-xe^{-x})}{x}\right)^2 + \frac{Z^2}{R}. \end{aligned} \tag{5}$$

where $x := RLZ$; note that $-xe^{-x} \geq -e^{-1}$, for all $x \geq 0$. The corresponding eigenfunctions can also be computed explicitly, cf. [1]. The ground state energy of h_δ is e_0, and the molecule will bind iff $\inf_R \left[e_0(R,L,Z) - e_{\rm at}\right] < 0$, where $e_{\rm at} = -Z^2L^2/2$, the ground state energy when the two nuclei are at infinite distance. The equilibrium distance $r_{\rm eq}$ is the value of R for which $e_0(R,L,Z) - e_{\rm at}$ is minimized. The following theorem summarizes the situation for the δ-model (numerical values are given to 4 decimal places):

Theorem 2. *(cf.* [2]*) The energy curve $e_0(R,L,Z) - e_{\rm at}$ has:*
(i) a global strictly negative minimum if $Z/L \leq 0.3205$;
(ii) has a local minimum (corresponding to a resonance of the molecule) if $0.3205 < Z/L < 0.4398$ and
(iii) does not have a local minimum if $Z/L > 0.4398$

To find the equilibrium distance, one computes that $\partial_R e(R,L,Z) = R^{-2}LZ\left[G(x) - ZL^{-1}\right]$, where $G(x) := x^{-1}(1+W)^{-1}(x+W)^2\,W$, where $W = W(xe^{-x})$. The function $G(x)$ is found to be strictly increasing on the interval $[0, x_G]$ where $G(x_G) = 0.4398$. Hence $r_{\rm eq} = G^{-1}(Z/L)$ for

$Z/L < 0.4398$. The ground state energy of molecule in the h_δ-model is $e_{\min} = e(r_{\rm eq}, L, Z)$. Their asymptotic behavior as $L \to \infty$ is given by:

$$r_{\rm eq} = \frac{1}{2L^{3/2}\, Z^{1/2}} \left(1 + \frac{5}{4}\theta + \frac{45}{32}\theta^2 + O(\theta^3)\right), \tag{6}$$

$$e_{\min} = -\, 2Z^2 L^2 \left(1 - 2\theta + \frac{5}{4}\theta^2 + O(\theta^3)\right), \tag{7}$$

where $\theta = \sqrt{Z/L}$. Although h_δ does not, by itself, provide numerically very good approximations for the ground-state energy and equilibrium distance of the real H_2^+-molecule for magnetic fields in the physically relevant range of $3\times 10^9 - 4\times 10^{13}$ Gauss, it can be used as the starting point of a perturbative calculation, as was done in [1]. The equilibrium distance and binding energy of the H_2^+ molecule computed there were found to be in good agreement with earlier variational calculations. One consequence of these computations is the prediction of the existence, in fields $B \geq 10^{13}$ G, of He_2^{3+}, a new atomic system, and a further example of the binding-enhancing properties of strong magnetic fields.

3 Equilibrium nuclear separation for H_2^+

Using the arguments of [5], section 9, it can be shown that the ground state energy $E_0 = E_0(R, L, Z)$ of H can be estimated in terms of that of h_δ by

$$|E_0(R, L, Z) - e_0(R, L, Z)| \leq c_\delta L,$$

uniformly in R (recall that the constant c_δ of theorem 1 is independent of R). One encounters a technical difficulty due to the existence of the second eigenvalue e_1 of h_δ which, for large fields, becomes exponentially close to e_0, and prohibits a lower bound for the isolation distance of e_0 of the type required for theorem 1. However, all Hamiltonians under consideration commute with the z-parity operator $P_z : z \to -z$, and if we decide right from the start to work in the $P_z = 1$-eigenspace of even functions in z, e_1 will not exist, and one can proceed as before. Using this estimate of $|E_0 - e_0| < c_\delta L$ and the fact that $e_0(L, Z, R)$ has a global minimum of order $\mathcal{O}(-L^2)$ if $Z/L \leq 0.3205$, one then shows, for sufficiently large B (and L), that the equilibrium distance $R_{\rm eq}$ of the true molecule (1) lies between the two roots $R = R_1$ and $R = R_2$ of the equation

$$e_{\min} + c_\delta\, L = e(R, L, Z) - c_\delta\, L\ . \tag{8}$$

A detailed analysis of this equation, using the known asymptotic large L-behavior of $e(R, L, Z) = x^{-1}L^2Z^2\,(L^{-1}Z - 2x + 4x^2 - 10x^3 + \mathcal{O}(x^4))$, $x =$

RLZ, and of $e_{\min}$ then shows that $R_{1,2} = (2L^{3/2}Z^{1/2})^{-1} + \mathcal{O}(L^{-7/4})$ (cf. [2], section 3). Hence:

Theorem 3. *For sufficiently large B, ground state energy and equilibrium distance of the H_2^+-molecule (1) is given by, respectively*

$$E_0(L, Z) = -2L^2Z^2 + 4Z^{5/2}L^{3/2} + \mathcal{O}(L), \tag{9}$$

and

$$R_{\text{eq}} = \frac{1}{2L^{3/2}\,Z^{1/2}} + \mathcal{O}\left(L^{-7/4}\right). \tag{10}$$

4 Discussion

By theorem 3, the internuclear distance tends to 0 as $B \to \infty$. Despite the electrostatic repulsion between the two nuclei, a single electron suffices, under the influence of a strong magnetic field, to bring them arbitrarily close to each other. This is again an example of the binding-enhancing effect of strong magnetic fields. Furthermore, as $B \to \infty$, $e_{\min} \to -2Z^2L^2$, which is the ground-state of $\frac{1}{2}p_z^2 - 2ZL\delta(z)$, a one-dimensional He^+-like ion with δ-potentials. By [5], section 9, the ground-state $E_0^{He^+}(B)$ of the true He^+-ion in a strong magnetic field will lie within a distance of $\mathcal{O}(L)$ of $-2Z^2L^2$. It follows therefore that

$$\frac{E_0^{\mathrm{H}_2^+}(B)}{E_0^{\mathrm{He}^+}(B)} \to 1, \quad B \to \infty. \tag{11}$$

The conclusion is that as field strength increases, the H_2^+-model goes over into its United Atom Limit, the He^+-ion. Several caveats are of course in order here. First of all, for values of $B \geq 4 \times 10^{13}$ Gauss, for which the electron's rest-mass becomes larger or equal than the lowest Landau level, our non-relativistic model should be replaced by a relativistic one (and ultimately of course nuclear effects will start to play a role). Next, the fixed-nuclei approximation is not realistic, and vibrational, and possibly also rotational, motions should be taken into consideration.

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Chapter 5

Conclusion

This thesis was devoted to the study of two quantum mechanical systems. For both systems, results in the form of published papers were obtained. The list of publications follows at the the end of this section, together with the list of citations.

Chapter 3 concerned the Aharonov-Bohm effect. First, the definition of the effect was introduced, followed by a short overview of its history and of some consequences it has in quantum theory. A definition of the system describing the effect was discussed with an emphasis on the choice of boundary conditions. A review of the literature was provided, focused on the idealized Aharonov-Bohm effect and its description by operators with singular potentials. Finally, the idealized Aharonov-Bohm effect on the background of a homogeneous magnetic field was investigated in detail.

Chapter 4 concerned matter in strong magnetic fields. The strong magnetic field regime was briefly described and its consequences for behavior of matter was mentioned. The approximative method introduced by [BD3] was explained in detail, and systems describing H_2^+ molecule were established. Finally, some properties of H_2^+ molecule in the presence of strong magnetic fields were investigated using the aforementioned method.

Aharonov-Bohm effect with a homogeneous magnetic field

In Chapter 3, a rigorous analysis of the system describing the idealized Aharonov-Bohm effect in the presence of a homogeneous magnetic field was provided. In some sense, it was a follow-up to the previous papers [DŠ] and [AT] where the pure idealized Aharonov-Bohm effect was studied. The method for defining the operators with point interaction, based on the theory of self-adjoint extensions and described in [AGHKH1], was used. The results

were the following.

The most general admissible family of Hamiltonians describing the system was properly defined. The operators were characterized by boundary conditions at the position of singularity. The spectrum of the standard Hamiltonian was defined explicitly, showing the splitting of the Landau levels and giving rise to finitely degenerated eigenvalues in each gap. The spectral properties of general Hamiltonians were investigated. Some particular cases were again solved explicitly. For the general case, the number of newly arising eigenvalues was computed. The Green function for the standard Hamiltonian was found.

H_2^+ molecule in a strong magnetic field

In Chapter 4, H_2^+ molecule in a strong magnetic field was analysed. The method of [BD3] was deployed, and a one-dimensional operator h_δ with point interactions was established. This explicitly solvable model, serving as an approximation of the original Hamiltonian H for large values of the magnetic field B, was then used to compute some basic properties of the molecule. The results were the following.

The convergence theorem for the operator h_δ was established, including the bound on the error estimate. The conditions for stability, resonance and instability of the molecule were derived in terms of the nuclei charge and the magnetic field. The asymptotic behavior of the ground state energy and the equilibrium distance were computed.

List of publications

[1] P. Exner, P. Šťovíček, and P. Vytřas, *Generalized boundary conditions for the Aharonov-Bohm effect combined with a homogenous magnetic field*, J. Math. Phys. **43** (2002), 2151–2168.

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