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HABILITAČNÍ PRÁCE

**Quantum Hamiltonians with magnetic fields:
effective dynamics and transport properties**

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ABSTRAKT V ČESKÉM JAZYCE

Kvantové hamiltoniány s magnetickým polem: efektivní dynamika a transportní vlastnosti

Tato práce pojednává o nerelativistických i relativistických kvantových hamiltoniánech s magnetickým polem pro částici vázanou na nadplochu či její trubcovité okolí. V nerelativistickém případě uvažujeme magnetický laplacián, v relativistické situaci potom Diracův operátor s magnetickým polem. Nejprve budeme hledat efektivní operátor pro magnetický laplacián na velice tenkém okolí nadplochy. Ukážeme, že jde-li šířka okolí k nule, je limitním operátorem magnetický Laplace-Beltramiho operátor na nadploše s dodatečným skalárním potenciálem, který lze zapsat pomocí hlavních křivostí nadplochy. Je-li nadplocha vložena do \mathbb{R}^3 , potom efektivní magnetické pole je dáno projekcí vnějšího magnetického pole do směru jednotkové normály k nadploše. Speciálně se dále zabýváme dvourozměrným magnetickým laplaciánem. Pro řadu translačně invariantních magnetických polí lze ukázat, že spektrum tohoto operátoru je čistě absolutně spojitě. Ukážeme, že tato vlastnost může zůstat zachována i po přičtení translačně invariantního elektrostatického potenciálu. Absolutní spojitost spektra dokážeme i pro magnetický laplacián s konstantním magnetickým polem na okolí zakřivené translačně invariantní dvourozměrné nadplochy. Připomeňme, že absolutní spojitost spektra bývá spojována s transportními vlastnostmi modelu. Navíc pro mnoho dvourozměrných modelů s translačně invariantní magnetickou bariérou byl odvozen dolní odhad pro velikost proudů podél bariéry. Ukážeme, že nosiči těchto proudů mohou být stavy s malou či nulovou disperzí a nalezneme postačující podmínky pro jejich existenci v relativistickém případě. Je-li magnetická bariéra popsána vektorovým potenciálem, který je úzkého vysokého profilu, jeví se jako smysluplné místo něj formálně uvažovat jednoduchou vrstvu. Přitom vzhledem k translační invarianci lze po zapojení částečné Fourierovy transformace pracovat s jednorozměrnými Diracovými operátory. Dává tedy smysl zabývat se jednorozměrnou relativistickou bodovou interakcí a jejími aproximacemi pomocí více realistických regulárních potenciálů. Aproximační výsledek odvodíme v uniformním rezolventním smyslu pro libovolný typ bodové interakce. Nakonec rigorózně definujeme dvourozměrný Diracův operátor s potenciálem úměrným jednoduše vrstvě na uzavřené křivce jako samosdružený operátor a analogicky jako v jednorozměrné situaci vyřešíme otázku aproximací pomocí regulárních potenciálů. Detailněji se budeme věnovat případu, kdy je možno singulární potenciál interpretovat jako vektorový potenciál, tj. nově zavedeme magnetickou δ -shell interakci.

ABSTRACT IN ENGLISH

Quantum Hamiltonians with magnetic fields: effective dynamics and transport properties

This thesis deals with both non-relativistic and relativistic quantum Hamiltonians with magnetic fields constrained to a hypersurface or its tubular neighbourhood. In the non-relativistic case, the magnetic Laplacian will be considered, whereas in the relativistic situation we will be concerned with the Dirac operator with magnetic field. Firstly, we will look for an effective operator for the magnetic Laplacian on a very thin neighbourhood of the hypersurface. We will show that, as the width of the neighbourhood tends to zero, the limit operator is the magnetic Laplace-Beltrami operator on the hypersurface with an additional scalar potential, which may be expressed in terms of the principal curvatures of the hypersurface. If the hypersurface is embedded into \mathbb{R}^3 then the effective magnetic field is given as the projection of the ambient magnetic field to the normal direction. Next, we will focus on the two-dimensional magnetic Laplacian. It has been proved for a variety of translationally invariant magnetic fields that the spectrum of this operator is purely absolutely continuous. We will show that this still may be true even after adding a translationally invariant electrostatic perturbation. Moreover, we will prove the absolute continuity of the Laplacian with constant magnetic field on neighbourhoods of certain curved translationally invariant two-dimensional hypersurfaces. Recall that the absolutely continuous spectrum is typically associated with transport properties of a model. Besides, for many two-dimensional models with a translationally invariant magnetic barrier, there exists a lower bound on currents along the barrier. We will show that these currents may be carried by states that disperse slowly or not at all and we will find several sufficient conditions for existence of such states in the relativistic case. If the vector potential that is associated with the magnetic barrier is of very thin but high profile, it seems reasonable to work formally with the simple layer distribution instead of the true, possibly complicated, potential. Moreover, due to the symmetry with respect to translations, it is possible to consider one-dimensional Dirac operators after employing the partial Fourier transform. Therefore, it makes sense to be concerned with the one-dimensional relativistic point interaction and its approximations by more realistic regular potentials. We will provide an approximation result in the norm resolvent sense for any type of the point interaction. Finally, we will introduce rigorously as a self-adjoint operator the two-dimensional Dirac operator with potential that is proportional to the simple layer distribution supported on a closed curve and, similarly as in the one-dimensional setting, we will solve the problem of approximations by regular potentials. We will investigate in more detail the case when the singular potential may be associated with a vector potential, i.e., we will introduce a sort of magnetic δ -shell interaction.

Chapter 1

Scope of the thesis

1.1 Introduction

The bible of modern mathematical physics by Reed and Simon [103] starts with an observation that "it is a common fallacy to suppose that mathematics is important for physics only because it is a useful tool for making computations". In fact, if a successful mathematical model is created to describe a physical phenomenon, it may be very fruitful to think about its mathematical structure, because understanding the mathematics of the model can largely extend our knowledge about the physics of the model or even lead to understanding of physical phenomena that were not originally described by the model. As a prominent example, one can recall Newtonian mechanics which was initially developed to describe the celestial motion but its model itself was used to describe almost all physical phenomena before the advent of the quantum physics, which became the central physical theory of 20th century and also these days. I dare to say that the role of mathematics in the quantum physics is even more important because the quantum physics deals with physical objects and phenomena that we do not experience directly by our human senses and classical analogies are often misleading.

The mathematical foundations of quantum mechanics were laid by John von Neumann to a large extent [93] with functional analysis being the key mathematical discipline. According to the axioms of quantum mechanics, observables are represented by self-adjoint operators in a Hilbert space of possible states. Prominent examples of these operators are the operators of the total energy, the so-called Hamiltonians, since they appear on the right-hand side of the Schrödinger and Dirac equations that govern the time evolution of a quantum state. This thesis deals with several non-relativistic and relativistic quantum Hamiltonians in the presence of magnetic fields. In particular, we will be concerned with the following questions.

Q1 Is it possible to describe the motion of a quantum particle constrained to a hypersurface by a Hamiltonian which is obtained as a certain limit of Hamiltonians on very thin tubular neighbourhoods of the hypersurface? What happens with an ambient magnetic field in this limit?

Q2 What are the effects of translationally invariant magnetic inhomogeneities in two-dimensional quantum systems? Is it possible to replace a magnetic inhomogeneity by a geometric deformation to get the same or similar effects?

Q3 What is an effective model for a two-dimensional quantum system with magnetic field that is associated with a vector potential which vanishes away from a very thin neighbourhood of a curve but is very large on this neighbourhood?

Most of these questions have longer or shorter history¹, thought in possibly slightly different settings, and are linked together. Moreover, although they lead to challenging problems in analysis of self-adjoint operators, they are not just mathematical curiosities. In fact, they were motivated by great achievements of the nano/meso-scopic physics and material sciences of recent decades.

After introducing the notion of magnetic Laplacian in Section 1.2, question **Q1** is addressed in Section 1.3. We will derive a norm resolvent convergence result in very general setting. Sections 1.4, 1.5, and 1.6 are devoted to problems related to question **Q2**. We will describe the effects of considered magnetic fields in terms of certain spectral quantities. First, we will study new sufficient conditions under which the spectrum of the associated magnetic Laplacian is purely absolutely continuous. Secondly, we will argue that the presence of energy bands in the spectrum of a quantum Hamiltonian guarantees the existence of quantum states that propagate with non-zero velocity and disperse only slowly or even not at all. As an example, we will study two-dimensional Dirac operator with magnetic fields. In Section 1.7, we will introduce the so-called magnetic δ -shell potential for the two-dimensional Dirac operator and show that it can be obtained as the strong resolvent limit of a sequence of two-dimensional Dirac operators with scaled vector potentials. This answers question **Q3** in the relativistic case. Comparing formal and mathematically rigorous limit operators we will observe a non-intuitive renormalization of the coupling constant. We will also discuss a similar one-dimensional model.

Notation

We will denote by $L^2(\Omega; \mathcal{H})$ the Hilbert space of the equivalence classes of almost everywhere identical square-integrable (with respect to the Lebesgue measure) functions on an open subset Ω of \mathbb{R}^n with values in a Hilbert space \mathcal{H} . If $\mathcal{H} = \mathbb{C}$ we will abbreviate $L^2(\Omega; \mathcal{H})$ to $L^2(\Omega)$. We will use similar conventions for all L^p -spaces, $p \in [1, \infty]$, and their subspaces. When convenient we will identify $L^2(\Omega; \mathbb{C}^2) \equiv L^2(\Omega) \otimes \mathbb{C}^2 \equiv L^2(\Omega) \oplus L^2(\Omega)$ and similarly for subspaces. The Sobolev space of the elements of $L^2(\Omega)$ that have all weak derivatives up to the order $m \in \mathbb{N}$, all of them being in $L^2(\Omega)$, will be denoted by $H^m(\Omega)$. We will write $H_0^m(\Omega)$ for the closure of $C_0^\infty(M)$, the space of all smooth functions with supports in M , with respect to the usual norm on $H^m(\Omega)$.

1.2 Magnetic Laplacian

In this section, we review some basic results about the self-adjointness and spectral properties of magnetic Laplacians. Let Ω be a domain, i.e., an open connected set, in \mathbb{R}^n . Note that later we will be mostly concerned with the case when $\Omega = \mathbb{R}^2$ or Ω is a tubular neighbourhood of a hypersurface in \mathbb{R}^n . The magnetic Laplacian acts on a subspace $\text{Dom}(H_A)$ of $L^2(\Omega)$ as follows

$$H_A = (-i\nabla + A)^2. \quad (1.1)$$

Here $A : \Omega \rightarrow \mathbb{R}^n$ is the vector potential. Since H_A (in appropriate units) should represent a quantum mechanical observable, $\text{Dom}(H_A)$ has to be chosen so that H_A is self-adjoint. There has been lot of effort to show self-adjointness of H_A under minimal assumptions on regularity of A . To this purpose it is convenient to start with the following quadratic form

$$q_A(\psi, \psi) = \|(-i\nabla + A)\psi\|_{L^2(\Omega)}^2$$

¹References will be provided later in separate sections.

defined initially for all $\psi \in C_0^\infty(\Omega)$. If $\Omega = \mathbb{R}^n$ and $A \in L_{\text{loc}}^2(\mathbb{R}^n; \mathbb{R}^n)$ then q_A is closable and its closure is the maximal form, i.e.,

$$\text{Dom}(\overline{q_A}) = \{\psi \in L^2(\mathbb{R}^n) \mid \|(-i\nabla + A)\psi\|_{L^2(\mathbb{R}^n)} < +\infty\},$$

cf. [71]. By representation theorem, there is a self-adjoint operator associated with $\overline{q_A}$. We will identify H_A with exactly this operator. Moreover, if $A \in L_{\text{loc}}^4(\mathbb{R}^n; \mathbb{R}^n)$ and $\nabla \cdot A \in L^2(\mathbb{R}^n)$ then H_A maps $C_0^\infty(\mathbb{R}^n)$ to $L^2(\mathbb{R}^n)$ and $C_0^\infty(\mathbb{R}^n)$ is an operator core of H_A [71]. Note that if A is differentiable and $A, \nabla A$ are bounded then the domain of H_A coincides with the domain of the free Laplacian H_0 , i.e., $\text{Dom}(H_A) = H^2(\mathbb{R}^n)$.

For bounded domains Ω (and similarly for unbounded domains with boundaries), there is no unique canonical way how to arrive at a self-adjoint realization of H_A . However, there are two realizations that appear almost exclusively in plenty of applications. For simplicity, let $A \in C^1(\overline{\Omega})$. The quadratic form q_A defined on the Sobolev space $H_0^1(\Omega)$ is closed and the associated self-adjoint operator $H_{A,D}$ is defined on

$$\text{Dom}(H_{A,D}) = \{\psi \in H_0^1(\Omega) \mid (-i\nabla + A)^2\psi \in L^2(\Omega)\}.$$

If we start with q_A defined on $H^1(\Omega)$ we get, using the representation theorem again, the self-adjoint operator $H_{A,N}$ acting on

$$\text{Dom}(H_{A,N}) = \{\psi \in H^1(\Omega) \mid (-i\nabla + A)^2\psi \in L^2(\Omega), (-i\nabla + A)\psi \cdot n = 0 \text{ on } \partial\Omega\},$$

cf. [98]. Here n stands for the outer normal to the boundary $\partial\Omega$ of Ω . Operators $H_{A,D}$ and $H_{A,N}$ are called the Dirichlet and Neumann realizations of the magnetic Laplacian, respectively, and act as the right-hand side of (1.1). Recall at this point that for sufficiently smooth boundaries, $\psi \in H^1(\Omega)$ belongs to $H_0^1(\Omega)$ if and only the trace of ψ on $\partial\Omega$ is zero.

Let us now introduce the notion of the magnetic field. We will assume that the vector potential $A \equiv (A_1, A_2 \dots A_n) : \Omega \rightarrow \mathbb{R}^n$ is C^1 -smooth. It gives rise to a 1-form $\alpha = A_i dx^i$. Here we used the Einstein summation convention and $\{x^i\}_{i=1}^n$ denote the Cartesian coordinates. The magnetic field is defined as the antisymmetric 2-form $\beta = d\alpha$. Remark that if χ stands for a differentiable scalar function then

$$d(\alpha + d\chi) = d\alpha = \beta.$$

Therefore, starting with a fixed magnetic field we have a certain freedom in the choice of the vector potential. This is well known change of gauge. On the other hand, if $d\alpha = d\tilde{\alpha}$, where $\tilde{\alpha}$ is another vector potential and Ω is such that we can use the Poincaré lemma (e.g., contractible) there exists a function χ such that $\tilde{\alpha} = \alpha + d\chi$. Physical quantities, like energies of bound states, depend on A (or equivalently α) only via β . Indeed, for any $\chi \in H^1(\Omega; \mathbb{R})$, we get

$$e^{-i\chi}(-i\nabla + A)e^{i\chi} = -i\nabla + A + \nabla\chi.$$

Therefore, it follows that H_A and $H_{A+\nabla\chi}$ are unitarily equivalent, because

$$U^\dagger H_A U = H_{A+\nabla\chi} \tag{1.2}$$

with $U = e^{i\chi}$. This result is called gauge invariance. Note that we identify the vector potential $A + \nabla\chi$ with a 1-form $\alpha + d\chi$. Let us stress that there exists domains and forms on them such that $d\alpha = 0$ but there is no χ with the property that $\alpha = d\chi$, i.e., forms that are closed but not exact. Recall the exterior of infinitely extended cylinder and the Aharonov-Bohm potential as an iconic example [1]. Using the Hodge star operator in \mathbb{R}^2 and \mathbb{R}^3 , one can identify 2-forms with

scalars and 1-forms, respectively. We will denote the Hodge dual of β by B and call it magnetic field again. It is possible to recover usual formulae for the coordinates of B . Namely, we have

$$B \equiv \partial_1 A_2 - \partial_2 A_1 \quad \text{and} \quad B \equiv \nabla \times A,$$

in \mathbb{R}^2 and \mathbb{R}^3 , respectively. Nevertheless, the description of vector potentials and magnetic fields in terms of forms (written in some local coordinates) becomes indispensable when dealing with Riemannian manifolds.

A universal feature of the magnetic field is that it cannot decrease the energy of the system described by H_A . This principle is encoded in the so-called diamagnetic inequality that may be stated as follows. For any $A \in L^2_{\text{loc}}(\mathbb{R}^n, \mathbb{R}^n)$ and $\psi \in L^2(\mathbb{R}^n)$ such that $(-i\nabla + A)\psi \in L^2(\mathbb{R}^n; \mathbb{C}^n)$, we have $|\psi| \in H^1(\mathbb{R}^n)$ and

$$|\nabla|\psi|(x)| \leq |(-i\nabla + A)\psi(x)|$$

for a.e. $x \in \mathbb{R}^n$ [72]. Consequently, we get

$$q_0(|\psi|, |\psi|) \leq q_A(\psi, \psi),$$

which, in view of the min-max principle, implies $\min \sigma(H_0) \leq \min \sigma(H_A)$. Let us stress that the diamagnetic inequality is not true when the spin is introduced.

Finally, we will present several important spectral results for H_A when $\Omega = \mathbb{R}^2$. Many authors considered the case when the magnetic field B is asymptotically constant, i.e., $B(x, y) \rightarrow B_0 \in \mathbb{R}$ as $|(x, y)| \rightarrow +\infty$, where x and y stand for Cartesian coordinates in \mathbb{R}^2 . If $B_0 = 0$ then $\sigma(H_A) = \sigma_{\text{ess}}(H_A) = [0, +\infty)$ [90, 70]. Moreover, if B is short-range, i.e., $B(x, y) = \mathcal{O}(|(x, y)|^{-1-\delta})$ at infinity with $\delta > 0$, then the spectrum of H_A is purely absolutely continuous [58]. However, the character of the essential spectrum may be very different in the long-range case. One can even construct magnetic Laplacians with dense point spectra [90]. If $B_0 \neq 0$ then H_A has pure point spectrum

$$\sigma(H_A) = \sigma_p(H_A) = \{(2k + 1)|B_0|, k \in \mathbb{N} \cup \{0\}\}, \tag{1.3}$$

where all eigenvalues are of infinite multiplicity and are known as the Landau levels [59]. The situation when B is not asymptotically constant is not fully understood. Nevertheless, there is a seminal result by Iwatsuka that deals with the magnetic field that is invariant with respect to translations in one direction, say y . Then B may be viewed as function of variable x only. If the limits of $B = B(x)$ at $\pm\infty$ are different then the spectrum of H_A is purely absolutely continuous and it may contain gaps [60]. A precise formulation of the result will be given in Section 1.4 together with an overview of related results.

1.3 Quantum layers

In the previous section we introduced the magnetic Laplacian not only in the physical three-dimensional space, but also on two-dimensional domains. Such operators may serve as quantum Hamiltonians describing charge carriers in flat mesoscopic structures [57, 74]. Since the real structures are of very small but still non-zero width, a natural question arises whether it is possible to get two-dimensional operators as limits of three-dimensional operators acting on smaller and smaller neighbourhoods of the underlying structures. To answer the question we will first need some notation. We will consider much more general situation than just flat two-dimensional domains.

Let Σ be a hypersurface in \mathbb{R}^n with $n \geq 2$ and define its ε -neighbourhood

$$\Omega_\varepsilon := \{x_\Sigma + u \mid n \in \mathbb{R}^d \mid (x_\Sigma, u) \in \Sigma \times (-\varepsilon, \varepsilon)\}, \tag{1.4}$$

where n is a unit normal vector field of Σ and $\varepsilon > 0$. Next, we consider the magnetic Laplacian with Dirichlet boundary conditions on $\partial\Omega_\varepsilon$, which will be denoted by $H_{A,D}^\varepsilon$. It is natural to choose the Dirichlet boundary conditions, because they correspond to the "infinite potential" away from the neighbourhood. Finally, let A_{eff} be the projection of A on Σ and $h_{A_{\text{eff}},D}^\Sigma$ be the magnetic Laplace-Beltrami operator on Σ subject to the Dirichlet boundary conditions on $\partial\Sigma$ (if Σ is not complete). Recall that the magnetic Laplace-Beltrami operator acts as the usual Laplace-Beltrami operator after replacing derivatives with respect to local variables $-i\partial_\mu$ by their magnetic counterparts $(-i\partial_\mu + A_{\text{eff},\mu})$.

For $n = 2, 3$ and $A \equiv 0$, it was discovered already in 1970 that the formal limit of $H_{0,D}^\varepsilon$ is not just $h_{0,D}^\Sigma$ but there is an extra potential V_{eff} that depends explicitly on the principal curvatures of Σ [64]. The same was later observed in higher dimensions [114]. The first mathematically rigorous study of $H_{0,D}^\varepsilon$ for $n = 2$ appeared in 1995 [30] and started still ongoing interest in the research of quantum layers and quantum waveguides, i.e., quantum systems living on Ω_ε and tubular neighbourhoods of curves in \mathbb{R}^n , respectively. Let us list just a few contributions that are closest to the present setting but with no magnetic field, [23, 24, 40, 41, 68, 118, 119], see also the monograph [38] for further references. There are significantly less results in the magnetic case. Effective Hamiltonians for two and three-dimensional magnetic quantum waveguides were investigated in 2014 [65]. Almost simultaneously we published the first paper dealing with effective Hamiltonians for magnetic quantum layers [66] (see Section 2.1 for the full text). Note that in the two-dimensional space the notions of the waveguide and the layer coincide, so there is a certain overlap. Recently, an alternative way how to arrive at effective Hamiltonians both for waveguides and layers in a unified manner was discovered [47].

Our main result says that

$$H_{A,D}^\varepsilon - \left(\frac{\pi}{2\varepsilon}\right)^2 \xrightarrow{\varepsilon \rightarrow 0} h_{A_{\text{eff}},D}^\Sigma + V_{\text{eff}} \quad (1.5)$$

in the norm resolvent sense with

$$V_{\text{eff}} = -\frac{1}{2} \sum_{\mu=1}^{n-1} \kappa_\mu^2 + \frac{1}{4} \left(\sum_{\mu=1}^{n-1} \kappa_\mu \right)^2,$$

where $\{\kappa_\mu\}_{\mu=1}^{n-1}$ denote the principal curvatures of Σ . Let us stress that this result was novel even for $A \equiv 0$ because convergence in that strong topology hadn't been settled before in an arbitrary dimension. Note that the limit operator acts on a different Hilbert space than $H_{A,D}^\varepsilon$ and that the Hilbert space where $H_{A,D}^\varepsilon$ lives is ε -dependent. Therefore, in the schematic formula (1.5) we have to identify $H_{A,D}^\varepsilon$ with a unitarily equivalent operator acting in the Hilbert space of L^2 -functions on a layer of a fixed width and also identify the Hilbert space where the limit operator lives with the range of the projection (in the new ε -independent Hilbert space) onto the lowest Dirichlet eigenfunction in the transverse direction. During this procedure the coefficients of $H_{A,D}^\varepsilon$ become ε -dependent. This also roughly explains the need of subtracting the divergent term on the left-hand side of (1.5).

Observe that the effective potential V_{eff} is the same as in the non-magnetic case and that for $n = 2, 3$ it is always non-positive. The latter means that the limit operator comprises an attractive interaction that may produce bound states below the essential spectrum. In fact, for non-straight infinite strips ($n = 2$), this is always the case [30]. Our result suggest that one can eliminate these disturbing bound states by switching a magnetic field on, due to its repulsive (diamagnetic) effect. For $n = 2$ and ε fixed this had been previously studied in [36].

Finally, note that $h_{A_{\text{eff}},D}^\Sigma$ contains information about both intrinsic and extrinsic geometry of Σ . The latter is due to the way how A_{eff} is defined. This is best visualized for $n = 2$ when we

get for the effective magnetic field $B_{\text{eff}} = n \cdot B|_{\Sigma}$, i.e., only the projection of ambient magnetic field B to the normal direction plays a role in the limit.

1.4 Iwatsuka model

1.4.1 Classical two-dimensional case

In the previous section we justified that planar quantum models with magnetic fields may be viewed as limits of more realistic systems living on very thin layers. Now, we look more closely at an important example of such models, introduced in 1985 by Iwatsuka [60]. Let the magnetic field be a function of one variable, say x , only, $B = B(x)$. It is convenient to work in the Landau gauge,

$$A_x \equiv 0, \quad A_y(x, y) \equiv A_y(x) = \int_0^x B(t) dt, \quad (1.6)$$

because the magnetic Laplacian,

$$H_A = -\partial_x^2 + (-i\partial_y + A_y(x))^2,$$

is then unitarily equivalent to the direct integral of one-dimensional operators,

$$\mathcal{F}_{y \rightarrow \xi} H_A \mathcal{F}_{y \rightarrow \xi}^{-1} = \int_{\mathbb{R}}^{\oplus} H_A[\xi] d\xi,$$

where $\mathcal{F}_{y \rightarrow \xi}$ stands for the partial Fourier-Plancherel transform and

$$H_A[\xi] = -d_x^2 + (\xi + A_y(x))^2.$$

If $B \in L^\infty(\mathbb{R}; \mathbb{R})$ then $H_A[\xi]$ is essentially self-adjoint on $C_0^\infty(\mathbb{R})$ for every $\xi \in \mathbb{R}$ [71].

It is conjectured that the spectrum of H_A is purely absolutely continuous, whenever B is non-constant [25]. Recall that, from a physical perspective, the points of the absolutely continuous spectrum of a Hamiltonian are energies at which the system described by the Hamiltonian exhibits transport, see [19] for a possible mathematical explanation of this relationship. To get a feeling why the conjecture may be true, consider the case $B(x) = B_\pm \in \mathbb{R} \setminus \{0\}$ for all $\pm x > 0$ with $B_+ \neq B_-$. Then there are classical orbits that consist of semicircles of different radii on each of the half-planes. Such orbits clearly wander off to infinity. Of course, for many initial conditions, the classical orbits are just closed circles. On the other hand, quantum states are not strictly localized, so a quantum particle may still "feel" the magnetic step along $x = 0$. Above all, the conjecture was motivated by the Iwatsuka's result [60]. He proved the absolute continuity of H_A for magnetic fields that obey

CON1 $B \in C^\infty(\mathbb{R}; \mathbb{R})$, and there exist constants M_\pm such that $0 < M_- \leq B \leq M_+$

CON2 and either of the following holds

$$\begin{aligned} \text{CON2a} \quad & \limsup_{x \rightarrow -\infty} B(x) < \liminf_{x \rightarrow +\infty} B(x) \\ & \text{or } \limsup_{x \rightarrow +\infty} B(x) < \liminf_{x \rightarrow -\infty} B(x), \end{aligned}$$

CON2b B is constant for all $|x|$ sufficiently large but non-constant on \mathbb{R} , and there exists x_0 such that $B'(x_-)B'(x_+) \leq 0$ for all $x_- \leq x_0 \leq x_+$.

M. Măntoiu and R. Purice demonstrated in [79] that **CON2b** may be relaxed to

CON2c B is non-constant and there exists a point x_0 such that for all x_1, x_2 with $x_1 \leq x_0 \leq x_2$ one has either $B(x_1) \leq B(x_0) \leq B(x_2)$ or $B(x_1) \geq B(x_0) \geq B(x_2)$.

Note that there is also some overlap of **CON2c** with **CON2a**.

P. Exner and H. Kovařík proved that the spectrum of H_A is purely absolutely continuous for a large class of compactly supported variations of a constant non-zero magnetic field [37]. More concretely, they arrive at the following sufficient conditions,

CON3 $B(x) = B_0 + b(x)$, where $B_0 > 0$ and b is bounded, piecewise continuous and compactly supported

CON4 and either of the following holds

CON4a b is nonzero and does not change sign,

CON4b let $[a_l, a_r]$ be the smallest closed interval that contains $\text{supp } b$; there are $c, \delta > 0$ and $m \in \mathbb{N}$ such that $|b(x)| \geq c(x - a_l)^m$ or $|b(x)| \geq c(a_r - x)^m$ for all $x \in [a_l, a_l + \delta)$ or $x \in (a_r - \delta, a_r]$, respectively.

In [115] (see Section 2.2), I showed that it is possible to relax **CON1** and, more importantly, found sufficient conditions on absolute continuity of $H_A + W$, where W is an electric field which is, much like the magnetic field, assumed to be invariant with respect to translations in y -direction, $W(x, y) \equiv W(x)$. To state the result we will need some notation. For any $f \in L^\infty(\mathbb{R}; \mathbb{R})$, we put

$$\begin{aligned} \underline{f}_+ &= \sup_{a \in \mathbb{R}} \text{ess inf}_{t \in (a, +\infty)} f(t) & \bar{f}_+ &= \inf_{a \in \mathbb{R}} \text{ess sup}_{t \in (a, +\infty)} f(t) \\ \underline{f}_- &= \sup_{a \in \mathbb{R}} \text{ess inf}_{t \in (-\infty, a)} f(t) & \bar{f}_- &= \inf_{a \in \mathbb{R}} \text{ess sup}_{t \in (-\infty, a)} f(t). \end{aligned}$$

I proved that the spectrum of $H_A + W$ is purely absolutely continuous if $B, W \in L^\infty(\mathbb{R}; \mathbb{R})$ are such that either of the following holds

CON5a $\underline{B}_\pm > 0 \wedge \underline{B}_+ \geq \bar{B}_- \wedge (\bar{W}_- - \underline{W}_+ < \underline{B}_+ - \bar{B}_-)$,

CON5b $\underline{B}_+ > 0 \wedge \bar{B}_- < 0$.

The same is true if we interchange the \pm indices everywhere in **CON5a** and **CON5b**. Note that that we do not require positivity of B . In fact, in **CON5b** the magnetic field has to change its sign and in **CON5a** it may be negative on a compact subset of \mathbb{R} .

Similar models with electric potentials were studied before. If the magnetic field is constant $B(x, y) = B_0 > 0$ then we can choose $A = (0, B_0 x)$ and all fiber operators $H_A[\xi]$ are mutually uniformly equivalent. Moreover, $H_A[0]$ is the one-dimensional harmonic oscillator Hamiltonian. Using [104, Theorem XIII.85], we deduce immediately the aforementioned result that the spectrum of H_A with a constant non-zero magnetic field contains only eigenvalues of infinite multiplicity—the Landau levels (1.3). Since the magnetic Laplacian with constant magnetic field is known as the Landau Hamiltonian, we will write H_L instead of H_A for it. It was observed that $H_L + \omega^2 x^2$ with $\omega > 0$ is purely absolutely continuous and this property remains stable under adding perturbations of some type [34]. For $W = W(x)$ non-constant non-decreasing and bounded, it was proved that the spectrum of $H_L + W$ is also purely absolutely continuous, with a band structure [20]. We obtained a similar result for non-positive $W \not\equiv 0$ supported on the positive half-line [35] (see also Section 2.3). In fact, another new extension of the original sufficient conditions by Iwatsuka was presented in [35, Theorem V.1]. If $W = W(x)$ is periodic only the spectrum below a fixed energy (that depends on the strength of the magnetic field) was shown to be absolutely continuous [91].

Since each of **CON1**, **CON3**, **CON5a** or **CON5b** implies

$$\lim_{x \rightarrow \pm\infty} A_y(x) = +\infty, \tag{1.7}$$

$H_A[\xi]$ has compact resolvent under either of these conditions. Consequently, the spectrum of $H_A[\xi]$ consists solely of eigenvalues, say $\{\lambda_n[\xi]\}_{n \in \mathbb{N}}$. Moreover, it is rather straightforward to verify that $\{H[\xi]\}$ form an analytic family of type (B). In view of [104, Theorem XIII.86], to show the absolute continuity of H_A it is now sufficient to prove that each $\lambda_n[\xi]$ is simple and non-constant. The latter condition is hardest to verify. Typically one uses cleverly chosen comparison operators or the Feynman-Hellmann formula. The first approach yields asymptotic behaviour of the eigenvalues at $\xi = \pm\infty$ and it is particularly useful in situations when the magnetic field behaves differently at $\pm\infty$. The second approach gives the derivative of $\lambda_n[\xi]$ with respect to ξ and is usually applied when the magnetic field (as a function of one variable) is compactly supported. Note that the absence of eigenvalues in the spectrum of H_A was proved recently even for some magnetic fields that do not necessarily obey (1.7) [101]. In some particular situations, this may also imply that the spectrum of H_A is purely absolutely continuous.

1.4.2 Iwatsuka type effect in curved layers

We have seen in Section 1.3 that a quantum particle confined to a three-dimensional layer of a small width in an ambient magnetic field "feels" only the the projection of the field to the transverse direction, $B_{\text{eff}} = n \cdot B|_{\Sigma}$, where n is the unit normal field of the underlying surface Σ . This suggests that keeping the ambient field constant, $B = B_0 \neq 0$, one can produce effectively non-constant magnetic field by modifying the layer's geometry. If the layer is invariant with respect to the translations in one direction and it is not flat then it seems reasonable to expect the spectrum of H_A to be purely absolutely continuous, in view of the results of Iwatsuka and his followers. We studied such layers in [35], which is included in this thesis as Section 2.3, and proved absolute continuity of the spectrum under several additional conditions on Σ and/or the width of the layer, i.e., 2ε . Let us stress that we did not always assume ε to be very small. On the other hand, in the very definition (1.4) of the layer, one typically wants the mapping $(x_{\Sigma}, u) \mapsto x_{\Sigma} + un$ to be diffeomorphic which yields a certain upper bound on the layer's width.

To formulate our results, let us begin with some notation. Let $\Gamma : s \mapsto (x(s), z(s))$ be a curve in the xz -plane parametrized by its arc-length measured from a reference point on the curve and κ its signed curvature. We define the surface Σ as the image of $(s, y) \in \mathbb{R}^2 \mapsto (x(s), y, z(s))$ and the layer Ω_{ε} as its ε -tubular neighbourhood—see (1.4). Next, let us consider the Dirichlet magnetic Laplacian $H_{A,D}^{\varepsilon}$ on Ω_{ε} with $A = (0, B_0 x, 0)$, $B_0 > 0$. The corresponding magnetic field points in the direction of positive z -coordinate, $B = (0, 0, B_0)$. The operator $H_{A,D}^{\varepsilon}$ is unitarily equivalent to the operator that acts in (global) curvilinear coordinates $(s, y, u) \in \mathbb{R}^2 \times (-1, 1)$ on the layer of fixed width equal to 2,

$$H_{A,D}^{\varepsilon} \equiv -\partial_s f_{\varepsilon}(s, u)^{-2} \partial_s + (-i\partial_y + A_2(s, u))^2 - \varepsilon^{-2} \partial_u^2 + V(s, u),$$

where

$$f_{\varepsilon}(s, u) = 1 - \varepsilon u \kappa(s), \quad A_2(s, u) = B_0 \left(x(s) - \varepsilon u \frac{dz}{ds}(s) \right),$$

and V is a rather complicate function of f_{ε} and the curvature of Γ , which will be denoted by κ , together with its first and second derivatives. One can deduce that

$$\lim_{\varepsilon \rightarrow 0} f_{\varepsilon} = 1, \quad \lim_{\varepsilon \rightarrow 0} V = -\frac{\kappa^2}{4},$$

pointwise, and, after the appropriate identifications described at the end of Section 1.3,

$$H_{A,D}^{\varepsilon} - \left(\frac{\pi}{2\varepsilon} \right)^2 \xrightarrow{\varepsilon \rightarrow 0} h_{\text{eff}}^{\Sigma} := -\partial_s^2 + (-i\partial_y + B_0 x(s))^2 - \frac{\kappa^2(s)}{4}$$

in the uniform resolvent topology. The limit operator h_{eff}^Σ acts in the Hilbert space $L^2(\mathbb{R}^2, dsdy)$ as the Iwatsuka's Hamiltonian with an extra potential, which has been discussed above. Note that after applying the partial Fourier-Plancherel transform in y -variable, both operators $H_{A,D}^\varepsilon$ and h_{eff}^Σ decompose into direct integrals.

Our first sufficient condition on absolute continuity of $H_{A,D}^\varepsilon$ relies on the fact that the uniform resolvent convergence implies the convergence of eigenvalues. Consequently, if we know that the energy bands of the fiber operators of h_{eff}^Σ are non-constant, we can conclude the same for the energy bands associated with the fibers of $H_{A,D}^\varepsilon$. However, this works only for energies below arbitrarily chosen threshold shifted by the lowest Dirichlet eigenvalue in the transverse direction, $(\pi/(2\varepsilon))^2$, and all sufficiently small ε . Therefore, if Γ is such that **CON5a** or **CON5b** from Section 1.4.1 holds true for $B = B_0 dx/ds$ and $W = -\kappa^2/4$, then we deduce that for any $E > 0$ there exists ε_E such that the spectrum of $H_{A,D}^\varepsilon$ below $E + (\pi/(2\varepsilon))^2$ is purely absolutely continuous for all $\varepsilon \in (0, \varepsilon_E)$. Similarly, any new result on non-constancy of the energy bands of h_{eff}^Σ would yield a new sufficient condition on absolute continuity of $H_{A,D}^\varepsilon$ below any threshold.

Modifying [104, Theorem XIII.86] for the case when energy bands may be degenerate or cross each other and using carefully chosen comparison operators we deduced that the spectrum of $H_{A,D}^\varepsilon$ is purely absolutely continuous for

one-sided-fold layers, i.e., when $\lim_{s \rightarrow \pm\infty} x(s) = +\infty$ or $\lim_{s \rightarrow \pm\infty} x(s) = -\infty$ with no extra assumptions on the width of the layer, or

bent asymptotically flat layers, i.e., when $dx/ds = \alpha_\pm \in (0, 1]$ for all large enough positive and negative s , respectively, $\alpha_+ \neq \alpha_-$, and the width of the layer is restricted.

See Figures 1 and 2 in [35] (Section 2.3) that depict typical profiles of the considered layers.

It is also remarkable that one can observe a rather wild spectral transition for flat inclined layers, i.e., layers with $\Gamma(s) = (s \cos \gamma, s \sin \gamma)$, where $\gamma \in (-\pi/2, \pi/2]$ is the angle between B and n . If $\gamma \in (-\pi/2, \pi/2)$ then the spectrum of $H_{A,D}^\varepsilon$ consists of infinitely degenerate eigenvalues only, whereas for $\gamma = \pi/2$, i.e., for layers parallel to the magnetic field, we deduced that the spectrum of $H_{A,D}^\varepsilon$ is purely absolutely continuous. Moreover, in the latter case we have $\sigma(H_{A,D}^\varepsilon) = \sigma_{\text{ac}}(H_{A,D}^\varepsilon) = [\mu_1, +\infty)$ where μ_1 is the lowest eigenvalue of the Dirichlet realization of the differential expression

$$-\varepsilon^{-2} \partial_u^2 + B_0^2 \varepsilon^2 u^2$$

in $L^2((-1, 1), du)$.

Finally, let us note that we believe that our sufficient conditions on absolute continuity are probably far from being optimal. On the other hand, since the considered fiber operators are now partial differential operators (in variables (s, u)), the spectral analysis is much more demanding than in the case of the classical Iwatsuka model.

1.5 Magnetic transport

1.5.1 Edge states

In this section we will discuss effects of translationally invariant magnetic fields on propagation properties of two-dimensional electron gas. We will focus on single-particle states that are described by the magnetic Laplacian introduced in Section 1.4.1. There we were interested exclusively in absolute continuity of the Hamiltonian. Now, we will look closer at other quantities that characterize transport properties of the system in finer detail.

Let us start with a magnetic step, $B(x) = B_\pm \in \mathbb{R}$ for all $\pm x > 0$. As already noted in Section 1.4.1, for non-zero B_\pm such that $B_+ \neq B_-$, there are classical orbits that propagate

along the step, i.e., y -axis, to infinity. If $B_+B_- < 0$ then they are called snake orbits and they were used already in early 70's to describe electron transport in multi-domain ferromagnets by semi-classical approach [78]. The snake orbits and other classical paths were compared with their quantum mechanical counterparts from a physicist's point of view in [102]. A detailed mathematical study for the case $0 < B_- < B_+$ and also a smoothed version of the magnetic step was done by Hislop and Soccorsi [53]. They found a uniform lower bound for the so-called edge current J_y defined as the expectation of the y -component of the velocity operator,

$$J_y(\psi) := \langle \psi, \frac{i}{2}[H_A, y]\psi \rangle = \langle \psi, (-i\partial_y + A_y(x))\psi \rangle,$$

for all states ψ in the range of the spectral projector for H_A and certain subintervals of

$$((2n+1)B_-, (2n+1)B_+), \quad n \in \mathbb{N} \cup \{0\}. \quad (1.8)$$

These states are called edge states are localized close to the step. Note that the endpoints of (1.8) are Landau levels for B_{\pm} . The results obtained in [53] complement results of Dombrowski, Germinet, and Raikov who proved that the so-called edge Hall conductance is quantized for a family of Iwatuska-like models [28]. To get the above mentioned results on the edge currents and the localization of edge states it is crucial to understand the behaviour of underlying energy bands in detail. It was later studied even in situations when B_{\pm} are of different signs or one of them is zero [50].

The edge current is not bounded from below for states ψ in the range of the spectral projector for H_A and intervals containing the endpoints of (1.8) (or for subintervals of (1.8) being arbitrarily close to the endpoints). This was proved in [88] for a subclass of C^∞ -smooth magnetic fields such that B is increasing and $\lim_{x \rightarrow \pm\infty} B(x) = B_{\pm}$ with $0 < B_- < B_+$ and later for sufficiently regular magnetic fields obeying $B(x) = B_+$ on a neighbourhood of $+\infty$ [89]. Such states are referred to as the bulk states and in contrast to the edge states they are not localized (in x -variable) in general [88].

Originally, the edge and bulk states were investigated for models with boundaries, a half-plane being the most prominent example. Let $\Omega = \{(x, y) \in \mathbb{R}^2 \mid x > 0\}$ and $H_{A,D}$ be the Dirichlet realization of the magnetic Laplacian on Ω with $A = (0, B_0x)$, $B_0 \in \mathbb{R} \setminus \{0\}$. Such operator describes a charged particle confined to a half-plane (by a "hard wall" along $x = 0$) under influence of the perpendicular magnetic field B_0 . There exist arc-shaped classical orbits bouncing from the hard wall and wandering off to infinity. It is natural to call the quantum states that propagate similarly along the boundary $x = 0$ the edge states. The existence these current carrying states for $H_{A,D}$ perturbed by an impurity potential, which is small relative to the magnetic field strength, was showed rigorously by De Bièvre and Pulé [26]. This phenomenon was pointed out before by Halperin in his seminal work on the quantum Hall effect [48], cf. [69], too. Occurrence of edge states was also studied for a model with the hard wall, i.e., the Dirichlet boundary conditions, replaced by a potential wall [77, 42]. In [42] also more general geometries (with hard walls) than a half-plane were considered. Estimates on the edge currents along both potential and hard walls for different geometries together with a nice review of previous results may be found in [51] and [52]. Note that whenever a general impurity potential is considered, the translational symmetry is lost. Therefore, one can not use the approach described in the last paragraph of Section 1.4.1 to prove the absolute continuity of the magnetic Laplacian for a range of energies. Instead, Mourre's theory of positive commutators [92] is applied typically.

1.5.2 Dispersionless states

Let us now recall an alternative direct definition of the edge and bulk subspaces that was introduced in [26] for the particular case of the Dirichlet realization $H_{A,D}$ of the magnetic Laplacian

on a half-plane with a constant magnetic field $B_0 > 0$. Such operator is unitarily equivalent to

$$H_{\text{hw}} = \int_{\mathbb{R}}^{\oplus} H_{\text{hw}}[\xi] d\xi \quad \text{with} \quad H_{\text{hw}}[\xi] = -\partial_x^2 + (\xi - B_0 x)^2.$$

Here the subscript "hw" stands for "hard-wall" and the fiber operators act in $L^2((0, +\infty))$ with the Dirichlet boundary condition at $x = 0$. One can show that, for all $\xi \in \mathbb{R}$, the spectrum of $H_{\text{hw}}[\xi]$ consists of isolated non-degenerate eigenvalues $\lambda_n[\xi]$ with normalized eigenfunctions $\psi_n[\xi]$. It is now possible to introduce n th band subspace as

$$\mathcal{H}_n := \{f\psi_n[\xi] = f(\xi)\psi_n[\xi](x) \mid f \in L^2(\mathbb{R}, d\xi)\},$$

which is clearly an invariant subspace of H_{hw} . To understand better the dependence of $\lambda_n[\xi]$ and $\psi_n[\xi]$ on B_0 , it is convenient to scale x and ξ as follows

$$\tilde{x} := \sqrt{B_0}x, \quad \kappa := \frac{\xi}{\sqrt{B_0}}.$$

Then H_{hw} is unitarily equivalent to

$$B_0 \tilde{H}_{\text{hw}} = B_0 \int_{\mathbb{R}}^{\oplus} \tilde{H}_{\text{hw}}[\kappa] d\kappa \quad \text{with} \quad \tilde{H}_{\text{hw}}[\kappa] = -\partial_{\tilde{x}^2} + (\kappa - \tilde{x})^2.$$

If we denote $\alpha_n[\kappa]$ the n th eigenvalue of $\tilde{H}_{\text{hw}}[\kappa]$ then

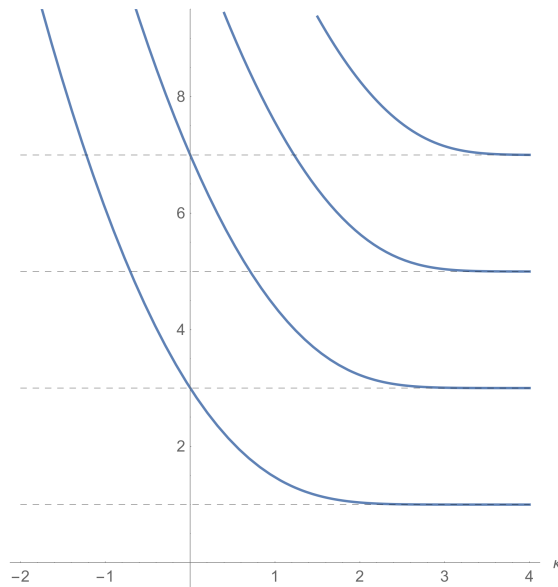


Figure 1.1: Four lowest energy bands $\alpha_n[\kappa]$, $n \in \{1, 2, 3, 4\}$ of \tilde{H}_{hw} .

$$\lambda_n[\xi] = B_0 \alpha_n\left[\frac{\xi}{\sqrt{B_0}}\right] \quad \text{and} \quad \frac{d}{d\xi} \lambda_n[\xi] = \sqrt{B_0} \frac{d}{d\kappa} \alpha_n\left[\frac{\xi}{\sqrt{B_0}}\right]. \quad (1.9)$$

Four lowest energy bands of \tilde{H}_{hw} , that were computed numerically, are depicted in Figure 1.1. By standard techniques for Schrödinger operators, it was deduced in [26] that $\frac{d}{d\kappa} \alpha_n[\kappa] = -|\frac{d}{dx} \tilde{\psi}_n[\kappa](0)|^2 < 0$, where $\tilde{\psi}_n[\kappa]$ is the eigenfunction of $\tilde{H}_{\text{hw}}[\kappa]$ associated with $\alpha_n[\kappa]$, and that

$\frac{d}{d\kappa}\alpha_n[\kappa]$ is exponentially small for large values of κ . Taking the second equation of (1.9) into account, this implies that, for all ξ 's of order $\sqrt{B_0}$ and smaller, $\frac{d}{d\xi}\lambda_n[\xi]$ is of order $\sqrt{B_0}$, whereas, for all ξ 's of strictly higher order than $\sqrt{B_0}$, $\frac{d}{d\xi}\lambda_n[\xi]$ is exponentially small. Therefore, it is natural to define the following subspaces of \mathcal{H}_n ,

$$\begin{aligned}\mathcal{H}_{n,e} &:= \{f\psi_n[\xi] \mid f \in L^2((-\infty, \sigma B_0^\gamma), d\xi)\} \\ \mathcal{H}_{n,b} &:= \{f\psi_n[\xi] \mid f \in L^2((\sigma B_0^\gamma, +\infty), d\xi)\},\end{aligned}$$

where $\sigma, \gamma > 0$. If $\gamma \leq 1/2$ then $\mathcal{H}_{n,e}$ is called an edge space and if $\gamma > 1/2$ then $\mathcal{H}_{n,b}$ is called a bulk space. Since $\frac{d}{d\xi}\lambda_n[\xi_0]$ is the group velocity in the y -direction of a wave packet $f\psi_n[\xi]$ with f supported close to ξ_0 and the currents carried by wave packets are proportional to their velocity, we see that this definition corresponds well to the description of the edge and bulk states given in Section 1.5.1.

We will now look closer at the time evolution of wave packets from the band spaces of a general quantum system possessing the translational symmetry. We will follow our paper [63], which is included as Section 2.4. For brevity, the problem will be described in the two-dimensional setting. Let a quantum Hamiltonian H in the Hilbert space $L^2(I \times \mathbb{R}, dx dy)$, where I is an open interval, be invariant with respect to translations in y -direction. Then we have

$$\mathcal{F}_{y \rightarrow \xi} H \mathcal{F}_{y \rightarrow \xi}^{-1} = \int_{\mathbb{R}}^{\oplus} H[\xi] d\xi,$$

where $H[\xi]$ acts in $L^2(I)$. Next, let us suppose that for open intervals J_n , $n \in 1, 2, \dots, N$ with $N \in \mathbb{N} \cup \{+\infty\}$, there exist eigenpairs of $H[\xi]$ denoted by the same symbols $\lambda_n[\xi]$ and $\psi_n[\xi]$ as in the special case discussed above, i.e., for all $\xi \in J_n$,

$$H[\xi]\psi_n[\xi] = \lambda_n[\xi]\psi_n[\xi].$$

Take $\beta_n \in L^2(\mathbb{R}, d\xi)$ such that $\text{supp } \beta_n \subset J_n$ and $\int_{J_n} |\beta_n(\xi)|^2 d\xi = 1$. If $\psi_n[\xi]$ are normalized to one then the same holds true for the wave packet

$$\Psi(x, y) := (\mathcal{F}_{y \rightarrow \xi}^{-1}(\beta_n(\xi)\psi_n[\xi](x)))(y),$$

which is just the Fourier preimage of a vector from the n th band subspace, so the following observations apply to the edge and bulk states introduced above. It is straightforward to verify that, for all $t \in \mathbb{R}$,

$$\int_{\mathbb{R}} |(e^{-itH}\Psi)(x, y)|^2 dy = \int_{\mathbb{R}} |\Psi(x, y)|^2 dy,$$

i.e., the probability density of finding a particle described by Ψ at distance x from the y -axis does not change with time. The dispersion of Ψ may be completely suppressed provided that the dispersion relation $\xi \mapsto \lambda_n[\xi]$ is linear,

$$\lambda_n[\xi] = e_n + v_n \xi,$$

since in that case one gets

$$(e^{-itH}\Psi)(x, y) = e^{-ite_n}\Psi(x, y - v_n t).$$

We see that the wave packet Ψ propagates along the y -axis with the uniform group velocity $v_n = \frac{d}{d\xi}\lambda_n[\xi]$.

If the dispersion relation is not linear but is close to linear (which can be achieved by considering β_n with a very narrow support) then Ψ disperse relatively slowly. For the speed of propagation of a dispersing wave packet we found a reasonably simple and accurate expression,

$$v = \frac{\int_{J_n} \frac{d\lambda_n}{d\xi} d\xi}{|J_n|} = \frac{\lambda_n[b] - \lambda_n[a]}{b - a}, \quad (1.10)$$

where $J_n = (a, b)$. Note that v is nothing but the averaged group velocity and the result is in a very good agreement with numerical examples, cf. Figure 2 in [63].

A natural question arises whether there are models of quantum systems with a linear band in the spectrum of their Hamiltonians. So far, we are only aware of few of them. Gruber and Leitner found linear bands in the spectrum of the two-dimensional Dirac operator on a half-plane with self-adjoint boundary conditions [46]. A linear band was also observed for a model of graphene with the so-called domain walls [107], the corresponding Hamiltonian being just 4×4 matrix two-dimensional Dirac operator with non-constant translationally invariant "mass term" $m = m(x, y) \equiv m(x)$ such that $\lim_{x \rightarrow \pm\infty} \pm m(x) = m_0$ with some $m_0 > 0$. Interestingly, if $m(x)$ is proportional to $\tanh(x)$ then the model is exactly solvable [87, 61, 63]. Finally, we recently studied the two-dimensional Dirac operator with the electrostatic δ -shell potential supported on a straight line [12]. If one adds the so-called magnetic δ -shell potential then it is possible to generate linear bands by fine tuning of coupling parameters—we are currently preparing a paper on this topic. All these Hamiltonians are relativistic. This is not surprising, because we are looking for systems whose energy depends linearly on ξ which is just the canonical momentum in y -direction.

1.6 Dirac operator with magnetic barrier

With enormous recent progress in understanding and preparation of the Dirac materials, the graphene being the most prominent example, there appeared a huge amount of physical papers dealing with the two-dimensional Dirac operator with magnetic barriers. There is no hope to provide a complete list of references. Let us just mention few of them that are close to our setting, [99, 75, 76, 94, 45, 100, 67, 83, 97, 73, 105, 112]. Since the dispersionless and slowly-dispersing states are associated with energy bands, it is desirable to know for which magnetic barriers there are bands in the spectrum of the associated Hamiltonian. In [39] (see Section 2.5 for the full text of the paper), we found several sufficient conditions for existence of energy bands in the spectrum of the two-dimensional Dirac operator D_A with a magnetic field possessing translational symmetry in one direction.

Working in the Landau gauge (1.6) again, D_A acts as follows

$$D_A = \sigma_1(-i\partial_x) + \sigma_2(-i\partial_y + A_y(x)) + \sigma_3 m$$

in the Hilbert space $L^2(\mathbb{R}^2; \mathbb{C}^2) \equiv L^2(\mathbb{R}^2; \mathbb{C}) \otimes L^2(\mathbb{R}^2; \mathbb{C}) \equiv L^2(\mathbb{R}^2; \mathbb{C}) \otimes \mathbb{C}^2$. Here

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are the usual Pauli matrices and m is a positive constant. We will assume in this section that the real function A_y is continuously differentiable and

$$\lim_{x \rightarrow \pm\infty} A_y(x) = 0, \quad \lim_{x \rightarrow \pm\infty} A'_y(x) = \lim_{x \rightarrow \pm\infty} B(x) = 0.$$

Then D_A is self-adjoint on the Sobolev space $H^1(\mathbb{R}^2; \mathbb{C}^2)$, by the Kato-Rellich theorem and the fact that the free Dirac operator D_0 is well known to be self-adjoint on the same domain, cf. [113]. Similarly as for the magnetic Laplacian, we get

$$D_A = \mathcal{F}_{y \rightarrow \xi}^{-1} \int_{\mathbb{R}}^{\oplus} D_A[\xi] d\xi \mathcal{F}_{y \rightarrow \xi},$$

where

$$D_A[\xi] = \sigma_1(-i\partial_x) + \sigma_2(\xi + A_y(x)) + \sigma_3 m \quad (1.11)$$

acts in $L^2(\mathbb{R}; \mathbb{C}^2)$. The energy bands of D_A consist of eigenvalues of $D_A[\xi]$. Existence of these eigenvalues in the gap of the spectrum of $D_A[\xi]$, i.e., in the interval $(-\sqrt{\xi^2 + m^2}, \sqrt{\xi^2 + m^2})$, was investigated in [62] using some ideas of supersymmetric quantum mechanics [86] together with the minimax principle for semi-bounded operators. This relies on the fact that the square of D_A is a direct sum of two Schrödinger operators $d_{\pm}[\xi]$, where $d_+[\xi] = pp^* + m^2$ and $d_- = p^*p + m^2$ with $p := -i(\partial_x + \xi + A_y)$.

Using the main theorem of [62] we deduced several sufficient conditions for the discrete spectrum of $D_A[\xi]$ be non-empty, which are easy to verify, such as

- If there exists $x_0 \in \mathbb{R}$ such that for all $x < x_0$, $A_y(x) \geq 0$ or $A_y(x) \leq 0$, respectively, and A_y is not integrable on $(-\infty, x_0)$ then for any $\xi < 0$ or any $\xi > 0$, respectively, $D_A[\xi]$ has infinite number of discrete eigenvalues.
- If there exists $x_0 \in \mathbb{R}$ such that for all $x > x_0$, $A_y(x) \geq 0$ or $A_y(x) \leq 0$, respectively, and A_y is not integrable on $(x_0, +\infty)$ then for any $\xi < 0$ or any $\xi > 0$, respectively, $D_A[\xi]$ has infinite number of discrete eigenvalues.

On the other hand, we derived the following sufficient conditions for emptiness of the discrete spectrum of $D_A[\xi]$,

- If $A_y \geq 0$ then, for all $\xi \geq 0$, there are no discrete eigenvalues in the spectrum of $D_A[\xi]$.
- If $A_y \leq 0$ then, for all $\xi \leq 0$, there are no discrete eigenvalues in the spectrum of $D_A[\xi]$.

With the help of these and similar criteria one can show that the studied system may host slowly-dispersing states. If all bands are monotonous then v defined in (1.10) is of definite sign, and so there exist only unidirectional slowly-dispersing states. In the opposite case bidirectional transport is possible. We analysed existence of slowly-dispersing states together with their character (unidirectional/bidirectional) for several realistic magnetic fields. See [39, Table 1] for a tabular overview of such results for the magnetic field generated by a system of parallel wires that carry currents that sum to zero.

1.7 Dirac operator with δ -interaction

1.7.1 One-dimensional Dirac operator with point interaction

Choosing $A_y(x) = C_\varepsilon \Theta(x) \Theta(\varepsilon - x)$ in (1.11), where $C_\varepsilon, \varepsilon > 0$ and Θ is the Heaviside theta function, one arrives at a simple implicit formula for the eigenvalues of $D_A[\xi]$ [83]. If we put $C_\varepsilon = \varepsilon^{-1}$ then $\lim_{\varepsilon \rightarrow 0} A_y = \delta$ in the sense of distributions. The corresponding limit operator was formally derived and studied in [97]. It acts as the free Dirac operator but on functions obeying certain transmission condition at the interaction point $x = 0$. However, we will show below that taking the formal limit does not yield the correct coupling constant that appears in the transmission condition. Instead, a careful mathematically rigorous treatment is necessary.

We will approach the problem from other side—we will start by introducing the one-dimensional Dirac operator with the so-called point interaction and then we will address the question how to approximate such interaction by more realistic potentials.

Consider formal expressions

$$\mathcal{D} := \sigma_1(-i\partial_x) + \sigma_3 m, \quad \mathcal{D}_{\eta,\tau,\lambda,\omega} := \mathcal{D} + (\eta\sigma_0 + \tau\sigma_3 + \lambda\sigma_2 + \omega\sigma_1)\delta,$$

where $m, \eta, \tau, \lambda, \omega \in \mathbb{R}$ and σ_0 is the 2×2 identity matrix. Note that $\{\sigma_i\}_{i=0}^3$ constitute a basis of the space of 2×2 hermitian matrices. Therefore, any hermitian matrix may occur in front of the Dirac δ -function. We would like to introduce $\mathcal{D}_{\eta,\tau,\lambda,\omega}$ as a self-adjoint operator in $L^2(\mathbb{R}; \mathbb{C}^2)$. To this aim, we have to firstly define a product of a not necessarily smooth function with δ -distribution. For any test function φ and $\psi \in L^2(\mathbb{R}; \mathbb{C}^2)$ such that one-sided limits $\psi(0_-)$ and $\psi(0_+)$ exist we put

$$(\psi\delta, \varphi) := \frac{\psi(0_+) + \psi(0_-)}{2} \varphi(0) = \left(\frac{\psi(0_+) + \psi(0_-)}{2} \delta, \varphi \right).$$

If $\psi \equiv \psi_- \oplus \psi_+ \in H^1(\mathbb{R}_-; \mathbb{C}^2) \oplus H^1(\mathbb{R}_+; \mathbb{C}^2) \subset L^2(\mathbb{R}_-; \mathbb{C}^2) \oplus L^2(\mathbb{R}_+; \mathbb{C}^2) \equiv L^2(\mathbb{R}; \mathbb{C}^2)$ then one can understand $\psi(0_-)$ and $\psi(0_+)$ as the values of the continuous representatives of ψ_- and ψ_+ , respectively. For $\psi \in H^1(\mathbb{R}_-; \mathbb{C}^2) \oplus H^1(\mathbb{R}_+; \mathbb{C}^2)$, we have

$$\mathcal{D}\psi = \mathcal{D}\psi_- \oplus \mathcal{D}\psi_+ - i\sigma_1(\psi(0_+) - \psi(0_-))\delta.$$

If we want $\mathcal{D}_{\eta,\tau,\lambda,\omega}\psi$ to be in $L^2(\mathbb{R}; \mathbb{C}^2)$, the singular contributions have to cancel out. This yields

$$-i\sigma_1(\psi(0_+) - \psi(0_-)) + (\eta\sigma_0 + \tau\sigma_3 + \lambda\sigma_2 + \omega\sigma_1) \frac{\psi(0_+) + \psi(0_-)}{2} = 0,$$

which is convenient to rewrite as

$$(2i\sigma_1 - (\eta\sigma_0 + \tau\sigma_3 + \lambda\sigma_2 + \omega\sigma_1))\psi(0_+) = (2i\sigma_1 + (\eta\sigma_0 + \tau\sigma_3 + \lambda\sigma_2 + \omega\sigma_1))\psi(0_-). \quad (1.12)$$

This motivates us to define the following operator

$$\begin{aligned} \text{Dom}(D_{\eta,\tau,\lambda,\omega}) &= \{\psi \equiv \psi_- \oplus \psi_+ \in H^1(\mathbb{R}_-; \mathbb{C}^2) \oplus H^1(\mathbb{R}_+; \mathbb{C}^2) \mid (1.12) \text{ holds}\} \\ D_{\eta,\tau,\lambda,\omega} &= \mathcal{D}\psi_- \oplus \mathcal{D}\psi_+. \end{aligned}$$

If the matrix on the left-hand side of (1.12) is invertible then we may further rewrite (1.12) as

$$\psi(0_+) = \Lambda\psi(0_-) \quad (1.13)$$

with

$$\Lambda := \frac{1}{d - (2i - \omega)^2} \begin{pmatrix} 4 + 4\lambda + \omega^2 - d & 4i(\tau - \eta) \\ -4i(\tau + \eta) & 4 - 4\lambda + \omega^2 - d \end{pmatrix},$$

where

$$d := \eta^2 - \tau^2 - \lambda^2. \quad (1.14)$$

This is exactly the transmission condition for the point interaction at $x = 0$ studied in [16]. An equivalent condition appeared before in [27] and some special cases were investigated even earlier in [44]. The operator $D_{\eta,\tau,\lambda,\omega}$ is self-adjoint and its spectral and scattering properties are very well understood, cf. [16, 21, 96].

To understand the nature of point interactions it is demanding to find approximating sequences with a clear physical interpretation. One is tempted to start with the following family of self-adjoint operators

$$\begin{aligned} \text{Dom}(D_{\eta,\tau,\lambda,\omega}^\varepsilon) &:= \text{Dom}(D_{0,0,0,0}) = H^1(\mathbb{R}; \mathbb{C}^2) \\ D_{\eta,\tau,\lambda,\omega}^\varepsilon &:= \mathcal{D} + (\eta\sigma_0 + \tau\sigma_3 + \lambda\sigma_2 + \omega\sigma_1)h_\varepsilon, \end{aligned}$$

where

$$h_\varepsilon(x) := \varepsilon^{-1}h(\varepsilon^{-1}x) \text{ for some } \varepsilon > 0 \text{ and } h \in L^1(\mathbb{R}; \mathbb{R}) \cap L^\infty(\mathbb{R}) \text{ such that } \int_{\mathbb{R}} h = 1, \quad (1.15)$$

because $h_\varepsilon \rightarrow \delta$ in the sense of distributions. It was demonstrated by Šeba [108] that $D_{\eta,0,0,0}^\varepsilon$ and $D_{0,\tau,0,0}^\varepsilon$ converge in the norm resolvent sense to $D_{\tilde{\eta},0,0,0}$ and $D_{0,\tilde{\tau},0,0}$, respectively, where the new coupling constants $\tilde{\eta}, \tilde{\tau}$ are non-trivial functions of h and are different from η, τ in general. This does not happen in the non-relativistic case, cf. [2]. In fact, a discrepancy between solving formally the Dirac equation with a δ -potential and solving it for a sequence of scaled short-ranged potentials and then taking the limit was observed before by physicists [84, 85]. The first approach was refused as unphysical, but we see that is perfectly admissible if one renormalizes the coupling constant properly.

Approximations for a general point interaction were studied by Hughes in the series of papers [55, 56]. However, she got convergence in the strong resolvent sense only. Recently, I proved the norm resolvent convergence for a three-parametric family of interactions [116] (see Section 2.6 for the full text of the paper) and my student Růžek completed the analysis by considering a general point interaction [106]. Moreover, I showed explicitly that the coupling constants must be renormalized, except for special cases, and that the limit coupling constants are independent of h as long as it integrates to a constant value. Note that this could have been deduced from the results of Hughes but it remained unnoticed for two decades. Here, we will present the approximation result in the same manner as in our very recent work [22] (see Section 3.1) on δ -shell interactions in two dimensions, which will be discussed in the next section. First, one can reduce the four-parametric family of point interactions to the three-parametric family with $\omega = 0$ by unitary equivalences. Then, for every $\eta, \tau, \lambda \in \mathbb{R}$ such that $d \notin \{(2k-1)^2\pi^2 \mid k \in \mathbb{N}\}$, $D_{\eta,\tau,\lambda,0}^\varepsilon$ converges in the norm resolvent sense to $D_{\tilde{\eta},\tilde{\tau},\tilde{\lambda},0}$ with

$$(\tilde{\eta}, \tilde{\tau}, \tilde{\lambda}) = \frac{\tan(\sqrt{d}/2)}{\sqrt{d}/2}(\eta, \tau, \lambda), \quad (1.16)$$

where d was defined in (1.14). If $d = 0$, we replace the factor in (1.16) by its limit, and for $d < 0$ we can choose either branch of the square root.

The approximation results justify why the interaction terms with coupling constants η and τ are referred to as the electrostatic and Lorentz scalar point interactions, respectively. The two remaining interaction terms were recently related to the magnetic interaction [22]. After "gauging away" the interaction term with the coupling parameter ω , which is a procedure that will be explained in the next section, we are left with the term $\lambda\sigma_2\delta$. By adding a symmetric bounded perturbation $\sigma_2\xi$, $\xi \in \mathbb{R}$, to $D_{0,0,\lambda,0}^\varepsilon$ we get exactly the fiber operator (1.11) of the two-dimensional Dirac operator with magnetic barrier, whose profile is given by $A_y = h_\varepsilon$. The corresponding limit operator is $D_{0,0,\tilde{\lambda},0} + \sigma_2\xi$ with $\tilde{\lambda} = 2 \tanh(\lambda/2)$, which is different from λ whenever $\lambda \neq 0$.

If the matrix on the left-hand side of (1.12) is not invertible, which happens if and only if $\omega = 0$ and $d = -4$, then one can show similarly as in [22, Lemma 5.1] that (1.12) is equivalent to a pair

of conditions that do not mix values $\psi(0_{\pm})$, i.e., the operator under consideration decouples into a direct sum of operators living on half-lines. These operators are also self-adjoint, as was proved in [46]. It is much more delicate task to find regular approximations in the decoupled case. Let us just mention that approximating potentials do not converge even in the distributional sense, cf. [106].

Finally, recall that Šeba also studied non-local approximations of the purely electrostatic and purely Lorentz scalar point interactions. For the purely electrostatic point interaction they were of the following form,

$$\mathcal{D} + \eta\sigma_0|h_{\varepsilon}\rangle\langle h_{\varepsilon}|.$$

As $\varepsilon \rightarrow 0$, this converges to $D_{\eta,0,0,0}$ in the norm resolvent sense [108], i.e., there is no renormalization of the coupling constant. Similar result holds for the Lorentz scalar point interaction, and my student Heriban proved the same for an arbitrary, not necessarily self-adjoint, point interaction [49]. This suggests that the nature of the relativistic point interactions may be non-local.

1.7.2 Two-dimensional Dirac operator with δ -shell interaction

The usual strategy how to add a point interaction to an essentially self-adjoint differential operator is to restrict its domain to the functions that vanish at the interaction point and then look for all possible self-adjoint extensions. There is a well known result by Svendsen [111] which implies that for n -dimensional Dirac operator the restriction itself is essentially self-adjoint whenever $n \geq 2$. Therefore, there is no point interaction for higher-dimensional Dirac operators. On the other hand, if we restrict the domain of the n -dimensional Dirac operator to the functions that vanish on a $(n-1)$ -dimensional smooth closed manifold Σ , the resulting operator has infinite deficiency indices. Thus, there exists a huge family of self-adjoint extensions, which are referred to as n -dimensional Dirac operators with δ -shell interaction.

As far as I know, the first mathematically rigorous study that deals with the relativistic δ -shell interaction is by Dittrich, Exner, and Šeba [27]. They considered the three-dimensional Dirac operator with δ -shell interaction supported on a sphere. The model was further analyzed in [29, 109, 81]. Of course, all these works are based on separation of variables. Self-adjointness and spectral properties for more general shells were derived relatively recently, firstly for the case of purely electrostatic δ -shell interaction [3, 4, 5, 8, 10], then for the purely Lorentz scalar δ -shell interaction [54], and finally for almost arbitrary combination of them [9], cf. also survey works [33] and [95]. The quasi-boundary triples, that were originally introduced to study elliptic differential operators [13], turned out to be very convenient tool when dealing with general shells. They just slightly generalize the concept of (ordinary) boundary triples from the extension theory, cf. [18].

In the two-dimensional setting, a general combination of the electrostatic and Lorentz scalar δ -shell interactions was introduced very recently by Behrndt, Holzmann, Ourmierès-Bonafos, and Pankrashkin [11]. They studied operators that act formally as

$$\mathcal{D}_{\eta,\tau}^{\Sigma} := \mathcal{D}_{2D} + (\eta\sigma_0 + \tau\sigma_3)\delta_{\Sigma},$$

where

$$\mathcal{D}_{2D} := \sigma_1(-i\partial_x) + \sigma_2(-i\partial_y) + \sigma_3m$$

and δ_{Σ} is the simple layer distribution supported on a smooth closed non-self-intersecting curve Σ in \mathbb{R}^2 , cf. [117]. Similarly as in Section 1.7.1, we deduce that if we want $\mathcal{D}_{\eta,\tau}^{\Sigma}f$ to be in $L^2(\mathbb{R}^2; \mathbb{C}^2)$ for a function f with suitably defined Dirichlet traces on both sides of Σ then

$$-in \cdot \sigma(\mathcal{T}_+f_+ - \mathcal{T}_-f_-) = \frac{1}{2}(\eta\sigma_0 + \tau\sigma_3)(\mathcal{T}_+f_+ + \mathcal{T}_-f_-). \quad (1.17)$$

Here $n = (n_1, n_2)$ is the unit normal field to Σ pointing outward the bounded domain Ω enclosed by Σ , $n \cdot \sigma := n_1\sigma_1 + n_2\sigma_2$, $f_+ := f|_\Omega$, $f_- := f|_{\mathbb{R}^2 \setminus \bar{\Omega}}$, and $\mathcal{T}_\pm f_\pm$ stand for the Dirichlet traces of f_\pm on Σ . Furthermore, for any open set $U \subset \mathbb{R}^2$, we introduce

$$H(\sigma, U) := \{f \in L^2(U; \mathbb{C}^2) \mid (\sigma_1 \partial_x + \sigma_2 \partial_y) f \in L^2(U; \mathbb{C}^2)\} = \{f \in L^2(U; \mathbb{C}^2) \mid \mathcal{D}_{2D} f \in L^2(U; \mathbb{C}^2)\}.$$

We are now ready to define the two-dimensional Dirac operator with the electrostatic and Lorentz scalar δ -shell interactions supported on Σ as

$$\begin{aligned} \text{Dom}(D_{\eta, \tau}^\Sigma) &:= \{f \equiv f_+ \oplus f_- \in H(\sigma, \Omega) \oplus H(\sigma, \mathbb{R}^2 \setminus \bar{\Omega}) \mid (1.17) \text{ holds true}\} \\ D_{\eta, \tau}^\Sigma &:= \mathcal{D}_{2D} f_+ \oplus \mathcal{D}_{2D} f_-. \end{aligned}$$

Self-adjointness of $D_{\eta, \tau}^\Sigma$ was basically proved by rewriting the transmission condition (1.17) in terms of operators Γ_0, Γ_1 of a cleverly chosen boundary triple $\{L^2(\Sigma; \mathbb{C}^2), \Gamma_0, \Gamma_1\}$ for $(D^\Sigma)^*$, where D^Σ acts as \mathcal{D}_{2D} on the domain $H_0^1(\mathbb{R}^2 \setminus \Sigma; \mathbb{C}^2)$, followed by showing self-adjointness of a certain boundary operator in $L^2(\Sigma; \mathbb{C}^2)$ [11]. Moreover, it turns out that in the so-called non-critical case, i.e., when $\eta^2 - \tau^2 \neq 4$, the functions in the domain of $D_{\eta, \tau}^\Sigma$ belong to $H^1(\mathbb{R}^2 \setminus \Sigma; \mathbb{C}^2)$. On the other hand, in the critical case, i.e., when $\eta^2 - \tau^2 = 4$, $\text{Dom}(D_{\eta, \tau}^\Sigma) \not\subset H^s(\mathbb{R}^2 \setminus \Sigma; \mathbb{C}^2)$ for any $s > 0$. In the non-critical case, $\sigma_{\text{ess}}(D_{\eta, \tau}^\Sigma) = \sigma_{\text{ess}}(D_{0,0}^\Sigma) = (-\infty, -|m|] \cup [|m|, +\infty)$ and the discrete spectrum in $(-|m|, |m|)$ is finite. The essential spectrum in the critical case differs from the essential spectrum in the non-critical case—it contains an extra value $-\tau m / \eta \in (-|m|, |m|)$. The key tool for spectral analysis is the Krein formula, an abstract version of the Birman-Schwinger principle.

Motivated by these results, we decided to study general δ -shell interactions [22] (see Section 3.1 for the full text of the manuscript), i.e., operators acting formally as

$$\mathcal{D}_{\eta, \tau, \lambda, \omega}^\Sigma := \mathcal{D}_{2D} + (\eta\sigma_0 + \tau\sigma_3 + \lambda t \cdot \sigma + \omega n \cdot \sigma)\delta_\Sigma,$$

where $t \equiv (t_1, t_2) = (-n_2, n_1)$ is the unit tangent field to Σ , $t \cdot \sigma := t_1\sigma_1 + t_2\sigma_2$, and $\eta, \tau, \lambda, \omega$ are smooth real functions on Σ . We define the operator $D_{\eta, \tau, \lambda, \omega}^\Sigma$ in the exactly same manner as the operator $D_{\eta, \tau}^\Sigma$ was defined, except for the transmission condition that now reads

$$-in \cdot \sigma (\mathcal{T}_+ f_+ - \mathcal{T}_- f_-) = \frac{1}{2}(\eta\sigma_0 + \tau\sigma_3 + \lambda t \cdot \sigma + \omega n \cdot \sigma)(\mathcal{T}_+ f_+ + \mathcal{T}_- f_-).$$

Extending ideas of [80], we proved that $D_{\eta, \tau, \lambda, \omega}^\Sigma$ is unitarily equivalent to $D_{X\eta, X\tau, X\lambda, 0}^\Sigma$ with an explicitly known constant X . Note that this result is always true for constant coupling parameters, but with non-constant coupling parameters we had to assume that at least ω and $d = \eta^2 - \tau^2 - \lambda^2$ remain constant along Σ in order to eliminate the coupling parameter ω . The involved unitary transform resembles U from the usual gauge invariance (1.2) but with a discontinuous gauge function. Having this sort of "gauge invariance" result in mind, we will further consider only the operators $D_{\eta, \tau, \lambda}^\Sigma \equiv D_{\eta, \tau, \lambda, 0}^\Sigma$. To prove their self-adjointness we had to modify the boundary triple introduced in [11]. In the present case, the non-critical case is characterized by the condition

$$\left(\frac{d}{4} - 1\right)^2 - \lambda^2 \neq 0 \quad \text{everywhere on } \Sigma. \quad (1.18)$$

Under this assumption we succeeded in proving self-adjointness of $D_{\eta, \tau, \lambda}^\Sigma$ and H^1 -regularity of the functions in the operator domain away from Σ .

If $d = -4$ everywhere on Σ then $D_{\eta, \tau, \lambda}^\Sigma$ decomposes into a direct sum of operators acting in $L^2(\Omega; \mathbb{C}^2)$ and $L^2(\mathbb{R}^2 \setminus \bar{\Omega}; \mathbb{C}^2)$, respectively. In the non-critical case, each of the operators is

self-adjoint. Therefore, this provides an alternative way how to show self-adjointness of the Dirac operator subject to a certain boundary conditions on a bounded domain Ω . In particular, for $\eta = 0$, one gets the so-called quantum dot boundary conditions, cf. [14, 15]. Note that one can get all quantum dot boundary conditions, except the zig-zag boundary conditions, by means of confinement with solely the electrostatic and Lorentz scalar δ -shell interactions [11]. Considering the magnetic δ -shell interaction ($\lambda \neq 0$) we can recover also the zig-zag boundary conditions, i.e.,

$$(\sigma_0 \pm \sigma_3)\mathcal{T}_+ f_+ = 0, \quad (1.19)$$

which correspond to the choice $(\eta, \tau, \lambda) = (0, 0, \pm 2)$. Beware that with this choice (1.18) is not valid, so we can not use our general self-adjointness result. Nevertheless, for $m = 0$, $D_{0,0,\pm 2}^\Sigma$ was proved to be self-adjoint employing the concept of supersymmetry [110]. The operators with $m \neq 0$ are just symmetric bounded perturbations of the operator with $m = 0$. Hence, their self-adjointness follows from the Kato-Rellich theorem. Spectral properties of $D_{0,0,\pm 2}^\Sigma$ may be describe in a fine detail. In particular, $\sigma(D_{0,0,\pm 2}^\Sigma) = (-\infty, -|m|] \cup [|m|, +\infty)$, $\pm m$ are eigenvalues of infinite multiplicity and beside them there is also a sequence of embedded eigenvalues derived from the eigenvalues of the Dirichlet Laplacian on Ω .

Beside generalizing the model considered in [11] in several directions, we found approximations of δ -shell interactions by means of scaled regular potentials. Let Ω_ε be the ε -tubular neighbourhood of Σ and h_ε be given as in (1.15) but with the extra assumption that $\text{supp } h \subset [-1, 1]$. If ε is below a certain threshold then for every $p \in \Omega_\varepsilon$ there is exactly one pair $(p_\Sigma, u) \in \Sigma \times (-\varepsilon, \varepsilon)$ such that $p = p_\Sigma + un(p_\Sigma)$. We are now ready to introduce a reasonable candidate for the approximating potential as

$$V_{\eta,\tau,\lambda;\varepsilon}(p) := \begin{cases} (\eta\sigma_0 + \tau\sigma_3 + \lambda t \cdot \sigma)(p_\Sigma)h_\varepsilon(u) & \text{if } p = p_\Sigma + un(p_\Sigma) \in \Omega_\varepsilon \\ 0 & \text{if } p \notin \Omega_\varepsilon. \end{cases}$$

Clearly, $V_{\eta,\tau,\lambda;\varepsilon} \xrightarrow{\varepsilon \rightarrow 0} (\eta\sigma_0 + \tau\sigma_3 + \lambda t \cdot \sigma)\delta_\Sigma$ in the sense of distributions. By the Kato-Rellich theorem, $D_{\eta,\tau,\lambda;\varepsilon}^\Sigma := \mathcal{D}_{2D} + V_{\eta,\tau,\lambda;\varepsilon}$ is self-adjoint on $H^1(\mathbb{R}^2; \mathbb{C}^2)$, which is the domain of self-adjointness of the two-dimensional free Dirac operator [113]. We proved that $D_{\eta,\tau,\lambda;\varepsilon}^\Sigma$ converges to $D_{\eta,\tilde{\tau},\tilde{\lambda}}^\Sigma$ with the coupling constants given in (1.16) in the strong resolvent sense as $\varepsilon \rightarrow 0$, whenever $d(p_\Sigma) \neq k^2\pi^2$, for all $k \in \mathbb{N}$, $p_\Sigma \in \Sigma$, and we are in the non-critical case with the limiting operator. Therefore, the same renormalization of the coupling constants as in the one-dimensional case is necessary.

In the three-dimensional setting only approximations for the purely electrostatic and purely Lorentz scalar interactions were studied so far by Mas and Pizzichillo [82]. They observed the same renormalization of the coupling constants as in the one-dimensional case, too. To prove the strong resolvent convergence they employed the Kato resolvent formula for the resolvent of the approximations and the Krein formula for the resolvent of the δ -shell interactions. At one point they had to assume a sort of smallness of the approximating potentials. In our proof, we decided to show the strong graph convergence, which is equivalent to the strong resolvent convergence in the self-adjoint setting. Beside being more direct, this approach does not yield any smallness restriction on the approximating potentials. Recall that the strong resolvent convergence implies that the spectrum of the limiting operator cannot suddenly expand in the sense that for any z in the spectrum of the limiting operator there is z_ε in the spectrum approximating operator such that $\lim_{\varepsilon \rightarrow 0^+} z_\varepsilon = z$ [103]. However, the spectrum of the limiting operator may contract in general. (This is not possible if one shows the norm resolvent convergence.) For spherical electrostatic δ -shell interaction it was proved that the point spectrum of the limiting operator does not contract [81].

Finally, let us look more closely at the purely magnetic δ -shell interaction. The formal expression for $D_{0,0,\lambda}^\Sigma$ is

$$\mathcal{D}_{2D} + \lambda t \cdot \sigma \delta_\Sigma = \sigma_1(-i\partial_x + \lambda t_1 \delta_\Sigma) + \sigma_2(-i\partial_y + \lambda t_2 \delta_\Sigma) + \sigma_3 m,$$

i.e., the term $\lambda t \cdot \sigma \delta_\Sigma$ corresponds to the singular vector potential $A_\Sigma = \lambda(t_1 \delta_\Sigma, t_2 \delta_\Sigma)$. This justifies why we call this term the magnetic δ -shell interaction. We will define the magnetic field B_Σ by exactly the same formula as in the regular case,

$$B_\Sigma = \partial_x A_{\Sigma,y} - \partial_y A_{\Sigma,x} = \lambda \partial_n \delta_\Sigma,$$

where $\partial_n \delta_\Sigma$ stands for the double layer distribution, cf. [117]. The vector potential and the corresponding magnetic field that appear in the approximating operator $D_{0,0,\lambda;\varepsilon}^\Sigma$ are given by

$$A_\varepsilon(p) = \begin{cases} \lambda h_\varepsilon(u) t(p_\Sigma) & \text{for } p = p_\Sigma + un(p_\Sigma) \in \Omega_\varepsilon \\ 0 & \text{for } p \notin \Omega_\varepsilon, \end{cases}$$

and

$$B_\varepsilon(p) = \begin{cases} \frac{\lambda h_\varepsilon(u) \kappa(p_\Sigma)}{1+u\kappa(p_\Sigma)} + \lambda h'_\varepsilon(u) & \text{for } p = p_\Sigma + un(p_\Sigma) \in \Omega_\varepsilon \\ 0 & \text{for } p \notin \Omega_\varepsilon, \end{cases}$$

respectively. Here, κ stands for the signed curvature of Σ . It is straightforward to show that $A_\varepsilon \xrightarrow{\varepsilon \rightarrow 0} A_\Sigma$ and $B_\varepsilon \xrightarrow{\varepsilon \rightarrow 0} B_\Sigma$ in the sense of distributions. However, according to our approximation result, $D_{0,0,\lambda;\varepsilon}^\Sigma$ converges to $D_{0,0,\tilde{\lambda}}$ in the strong resolvent sense, where $\tilde{\lambda}$ is always (except for the trivial case $\lambda = 0$) different from λ .

1.8 Future prospects

Self-adjointness of Dirac operators on domains has been understood only recently [14]. This is probably the reason why there are no rigorous mathematical studies concerning the relativistic counterparts of quantum waveguides and layers except for a recent preprint [17]. Therein, the two-dimensional Dirac operator constrained to a tubular neighbourhood Ω_ε of a curve Σ , cf. (1.4), was investigated. The Dirichlet boundary conditions, that are usual choice in the non-relativistic setting, would not yield a self-adjoint realization of the Dirac operator. However, it is known that the so-called infinite mass boundary conditions are right replacement for the Dirichlet ones [6, 7]. When ε tends to zero, the limiting operator for the Dirac operator on Ω_ε with the infinite mass boundary conditions is just the free one-dimensional Dirac operator (with the mass term being $2/\pi$ -multiple of the original mass term) [14]. Recall that in the two-dimensional non-relativistic setting there is always an attractive geometric potential in the limiting operator, cf. (1.5). Consequently, existence of bound states induced by geometry is a hallmark of non-relativistic quantum waveguides. In the relativistic setting, the limiting operator has purely absolutely continuous spectrum. Nevertheless, the question whether there are bound states for small but non-zero ε 's remains open. Beside studying relativistic quantum waveguides with the infinite mass boundary conditions in further detail, one should be concerned with other types of boundary conditions such as the zig-zag boundary conditions since they have been considered for graphene nano-ribbons by physicists [43, 32, 31]. In particular, a mathematical analysis of edge states would be desirable.

In Section 1.7.2, we briefly described how to introduce the two-dimensional relativistic δ -shell interactions supported on smooth closed curves. A more detailed analysis reveals that during the proof of self-adjointness using the boundary triples techniques one needs to show regularity

preserving properties of a certain boundary integral operator, cf. [11, Proposition 3.3]. This is done using the Cauchy transform and some pseudo-differential calculus on closed smooth curves. These tools are not available when we decide to deal with unbounded curves. However, for the special case of a straight line one can use the Fourier transform instead [12]. In fact, one can even consider compactly supported perturbations of the straight line. This will be explained in future work. Our final aim is to introduce any type of δ -shell interaction supported on a general unbounded curve. Note that even for the simplest example of such operator that is formally given by the differential expression

$$\mathcal{D}_{2D} + \eta\sigma_0\delta_\Sigma, \tag{1.20}$$

where Σ is a straight line and $\eta \neq 0$, we observed spectral effects that do not occur for interactions supported on closed curves. In particular, if $\eta \neq \pm 2$ then the spectrum of the self-adjoint realization of (1.20) is purely absolutely continuous and it is always strictly larger than the spectrum of the free Dirac operator, cf. [12, Theorem 1.1]. Therefore, playing with the parameter η , one can shrink the gap $(-|m|, |m|)$ in the spectrum of the latter operator. If $\eta = \pm 2$ then the absolutely continuous spectrum is stable but zero is an extra eigenvalue of infinite multiplicity.

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Chapter 2

Relevant published articles of the author

2.1 The magnetic Laplacian in shrinking tubular neighborhoods of hypersurfaces

What follows is a published article

D. Krejčířík, N. Raymond, and M. Tušek, The magnetic Laplacian in shrinking tubular neighborhoods of hypersurfaces, *J. Geom. Anal.* **25** (2015).

2.2 On an extension of the Iwatsuka model

What follows is a published article

M. Tušek, On an extension of the Iwatsuka model, J. Phys. A **49** (2016).

2.3 A geometric Iwatsuka type effect in quantum layers

What follows is a published article

P. Exner, T. Kalvoda, M. Tušek, A geometric Iwatsuka type effect in quantum layers, *J. Math. Phys.* **59** (2018).

2.4 Dispersionless wave packets in Dirac materials

What follows is a published article

V. Jakubský, M. Tušek, Dispersionless wave packets in Dirac materials, *Ann. Phys.* **378** (2017).

2.5 Qualitative analysis of magnetic waveguides for two-dimensional Dirac fermions

What follows is a published article

M. Fialová, V. Jakubský, M. Tušek, Qualitative analysis of magnetic waveguides for two-dimensional Dirac fermions, *Ann. Phys.* **395** (2018).

2.6 Approximation of one-dimensional relativistic point interactions by regular potentials revised

What follows is a published article

M. Tušek, Approximation of one-dimensional relativistic point interactions by regular potentials revised, *Lett. Math. Phys.* **110** (2020)

Chapter 3

Relevant preprint of the author

3.1 General δ -shell interactions for the two-dimensional Dirac operator: self-adjointness and approximation

What follows is a preprint

B. Cassano, V. Lotoreichik, A. Mas, M. Tušek, General δ -shell interactions for the two-dimensional Dirac operator: self-adjointness and approximation, <https://arxiv.org/abs/2102.09988> (2021).