Expansions in generalized eigenfunctions of Dirac operators

Thesis submitted in partial fulfillment of the requirements for the degree

Master of Science

Presented by

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under the supervision of
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Mathematatisches Institut der
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Abstract. [1] For the 2-dimensional massless Dirac operator with external potentials (which are allowed to explode at infinity) we find weighted Sobolev spaces where its generalized eigenfunctions lie. We also establish the relationship between the spectrum and the generalized eigenvalues. For the 1-dimensional massless Dirac operator we give an explicit expansion in generalized eigenfunctions and use it to show that the motion of massless Dirac particles is ballistic independently of the external potential.

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Ich erkläre hiermit, dass ich diese Master's Thesis selbständig und nur mit den angegebenen Hilfsmitteln angefertigt habe.

München, 9. August 2013

Table of contents

1. Introduction

Every self-adjoint operator in a finite-dimensional Hilbert space has a complete set of orthonormal eigenvectors, and therefore every element of the Hilbert space can be written as a linear combination of them –it has an *expansion* in eigenvectors–. This is a nice feature that one would like to have in the infinite-dimensional case[1.1]. It still holds in separable Hilbert spaces for self-adjoint operators with pure point spectrum, but fails with the presence of continuous spectrum. Even the self-adjoint operators associated to the most basic quantum observables position and momentum have no eigenvalues at all. But let us consider the momentum operator $p := -\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}x}$ in $L^2(\mathbb{R})$:

The functions $e_\lambda(x) := \frac{1}{\sqrt{2\,\pi}}\,\mathrm{e}^{\mathrm{i}\lambda x}$, although they are not eigenvalues since they are not L^2-functions, fulfill the relation $-\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}x} e_\lambda(x) = \lambda\, e_\lambda(x)$ for each $\lambda \in \mathbb{R} = \sigma(p)$, and via the inverse Fourier formula give an expansion for each $\psi \in L^2(\mathbb{R})$ in the sense

$$\psi(x) = \operatorname*{l.i.m.}_{N\to\infty} \int_{-N}^{N} e_\lambda(x)\,\hat{\psi}(\lambda)\,\mathrm{d}\lambda,$$

where

$$\hat{\psi}(\lambda) = \operatorname*{l.i.m.}_{N\to\infty} \int_{-N}^{N} \overline{e_\lambda(x)}\;\psi(x)\,\mathrm{d}x$$

denotes the Fourier transform of ψ.

This example suggests that enlarging the space of admisible eigenfunctions one could overcome the problem of the lack of eigenfunctions and obtain an expansion in *generalized eigenfunctions* also in the infinite-dimensional case.

The theory of generalized eigenfunctions has been developed separately for different settings. There are three main types of expansions in generalized eigenfunctions[1.2]:

- IP expansions (Ikebe [Ike60], Povzner [Pov55]) for Schrödinger operators with short-range potentials. These are very useful in scattering theory, for instance to prove asymptotic completeness of the wave operators and to give an expression of the scattering matrix (see [RS79, §XI.6]).

- Expansions for self-adjoint operators defined by symmetric ordinary differential expressions have been developed in [Wey10], [Kod50] and more recently treated in [Wei87].

- BGK expansions (Berezanskii, Browder, Garding, Gel'fand, Kac) were first proved to exist for elliptic differential operators with smooth coefficients [Ber68] and later for a variety of Schrödinger operators with singular potentials [KS78]. An approach to these expansions using the method in [Wei87, Chapter 8] for ordinary differential operators is given in [PSW89] and [PS93]. A remarkable consequence of the BKG expansions is that every point in the spectrum is arbitrarily close to a *generalized eigenvalue*. This fact together with the polynomial boundedness of the generalized eigenfunctions for Schrödinger operators was first used by Pastur [Pas80] and a few years later by Martinelli and Scoppola [MS85] to prove the absence of absolutely continuous spectrum for some random Schrödinger operators. This has played an important role for results on Anderson localization [FMSS85], [DK89]. Actually, for Schrödinger operators the relation $\sigma(H) = \overline{\{\lambda | Hu = \lambda\, u \text{ has a polynomially bounded solution}\}}$ holds, [Sim82, §C.4 and §C.5]. We shall prove the analogous statement for the Dirac operator.

1.1. It is in fact one of the assumptions in quantum mechanics [Sch68, §10].

1.2. We follow the classification in [PS93].

Here we focus in generalized eigenfunction expansions of the BGK type for Dirac operators. In §2 we introduce the theory on eigenfunction expansions following [PS93] for abstract self-adjoint operators and [Wei87] for ordinary differential operators. In §3 we study the 2-dimensional massless Dirac operator with electromagnetic potentials which are allowed to grow at infinity. We use the results in [PS93] to find weighted L^2 and H^1-spaces where its generalized eigenfunctions lie. We also establish the relationship between the spectrum and the generalized eigenvalues adapting Simon's proof for Schrödinger operators [Sim82, Theorem C.4.1]. In §4 we treat the 1-dimensional case. A clear advantage is that the powerful theory for ordinary differential operators is here applicable. We use the method in [Wei87, Chapters 9] to compute an expansion in generalized eigenfunctions of the 1-dimensional massless Dirac operator with external potential. We later use this expansion to study the dynamical behaviour of the massless Dirac particles, which is proved to be ballistic independently of the external potential. The Appendix contains some important results on operator theory with the purpose of making the reading easier.

1.1. Notation.

$\mathcal{D}(A)$ denotes the domain of the operator A and $\mathcal{R}(A)$ its range.
$\langle \mathbf{x} \rangle := (|\mathbf{x}|^2+1)^{1/2}$.
$L^p_s := \{\psi \colon \langle \mathbf{x} \rangle^s \psi \in L^p\}$, $H^k_s := \{\psi \colon \langle \mathbf{x} \rangle^s \psi \in H^k\}$.
$B_2(\mathcal{H})$ denotes the space of Hilbert-Schmidt operators in the Hilbert space $\mathcal{H}$.
χ_M or $\chi(M)$ denote the characteristic function of the set M.
Id denotes the identity function $\mathrm{Id}(x) = x$.
For the identity matrix we write $\mathbb{I}$ or simply 1.
The multiplication operator by a function h is also denoted by h.
Both $\mathcal{F}\psi$ and $\hat{\psi}$ denote the Fourier transform of ψ in L^2.
$[A, B] := A\,B - B\,A$ denotes the commutator of A and B on a suitable domain.
l.i.m. denotes the limit in L^2 of point-wise given functions. It stands for "limit in mean".

2. Expansions in generalized eigenfunctions

2.1. BGK expansions.

We introduce the concept of generalized eigenfunction and expansion in generalized eigenfunctions in the sense of BGK using the approach given in [PSW89] and [PS93]. As mentioned in the introduction in many cases the eigenfunctions of a self-adjoint operator are not enough to span the whole Hilbert space. Therefore one should generalize the definition of eigenfunction in order to have functions from outside of the space come into play. For a separable Hilbert space $\mathcal{H}$ we first present the construction of a Hilbert space-triple $\mathcal{H}_+ \subset \mathcal{H} \subset \mathcal{H}_-$, where the bigger space $\mathcal{H}_-$ will be the new space of admissible eigenfunctions.

Let $(\mathcal{H}, \langle\cdot,\cdot\rangle)$ be a separable Hilbert space and let T be a self-adjoint operator in $\mathcal{H}$ with $T \geqslant 1$. Then $\mathcal{D}(T)$ with the scalar product defined by $\langle u, v\rangle_+ := \langle Tu, Tv\rangle$ is a Hilbert space, which will be denoted by $\mathcal{H}_+(T)$. Since $0 \notin \sigma(T)$, the inverse $T^{-1}: \mathcal{H} \to \mathcal{D}(T)$ exists and $\langle \psi, \phi\rangle_- := \langle T^{-1}\psi, T^{-1}\phi\rangle$ defines another scalar product on $\mathcal{H}$. For the completion of $(\mathcal{H}, \langle\cdot,\cdot\rangle_-)$ we will write $\mathcal{H}_-(T)$. The triple $\mathcal{H}_+(T) \subset \mathcal{H} \subset \mathcal{H}_-(T)$ is called the ***T*-triple** of $\mathcal{H}$. It holds

Lemma 2.1. [PSW89, Lemma 1]

a) *Let $u \in \mathcal{H}_+(T)$, $\psi \in \mathcal{H}_-(T)$; for every sequence $(\psi_n) \subset \mathcal{H}$ with $\|\psi_n - \psi\|_- \to 0$ the limit $\langle \psi, u\rangle := \lim \langle \psi_n, u\rangle$ exists and it is independent of the choice of the sequence.*

b) *Let $\hat{T}$ be T considered as an operator with values in $\mathcal{H}_-(T)$; the closure $\tilde{T}$ of $\hat{T}$ is an isometric operator from $\mathcal{H}$ onto $\mathcal{H}_-(T)$.*

c) *For $u \in \mathcal{H}_+(T)$ and $\psi \in \mathcal{H}$ we have $\langle \tilde{T}\psi, u\rangle = \langle \psi, Tu\rangle$.*

Equivalently, one can define $\mathcal{H}_-(T)$ as the space of bounded linear functionals on $\mathcal{H}_+(T)$ with the functional norm $\|\cdot\|_-$. A detailed discussion is given in [Ber68, Chapter 1, §1].

We go back to the example in the introduction with the momentum operator $p = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}$ in $L^2(\mathbb{R})$, which via the Fourier transform $\mathcal{F}$ is unitarily equivalent to the multiplication by the identity ($\mathcal{F}p\mathcal{F}^{-1} = \mathrm{Id}$) in $L^2(\mathbb{R})$. For $e_\lambda(x) = (2\pi)^{-1/2}\mathrm{e}^{\mathrm{i}\lambda x}$ and $\langle f, g\rangle$ the pairing $\int \bar{f} g$ we have

a) For $\varphi \in C_0^\infty(\mathbb{R})$, $\mathcal{F}\varphi(\lambda) = \langle e_\lambda, \varphi\rangle$ a.e.

b) $\langle e_\lambda, p\varphi\rangle = \lambda\langle e_\lambda, \varphi\rangle$ for all $\lambda \in \mathbb{R}$ and $\varphi \in C_0^\infty(\mathbb{R}) \subset \mathcal{D}(p)$.

c) $\mathcal{F}^{-1}\phi = \lim_{N\to\infty}\int_{-N}^{N} e_\lambda\,\phi(\lambda)\,\mathrm{d}\lambda$
and
$\psi = \lim_{N\to\infty}\int_{-N}^{N} e_\lambda\,\mathcal{F}\psi(\lambda)\,\mathrm{d}\lambda$, for all $\phi, \psi \in L^2(\mathbb{R})$.

b) justifies the name of generalized eigenfunction for e_λ and c) specifies in which sense they give an expansion for each element in $L^2(\mathbb{R})$. The precise definitions of these concepts will be given via the next theorem, which generalizes this example for a large class of self-adjoint operators.

Theorem 2.2. [PS93, Theorem 2.2] *Let H be a self-adjoint operator in the separable Hilbert space $\mathcal{H}$, let (X, ρ) be a σ-finite measure space, $h: X \to \mathbb{R}$ a ρ-measurable function, and $U: \mathcal{H} \to L^2(X, \rho)$ a unitary operator such that*

$$UHU^* = h$$

(where h denotes also the multiplication operator by h). Write $X = \bigcup_{l=1}^{\infty} X_l$, with $X_l \subset X$ ρ-measurable, $\rho(X_l) < \infty$ and $X_l \subset X_{l+1}$ for every l. Let $\mathcal{H}_+(T) \subset \mathcal{H} \subset \mathcal{H}_-(T)$ be a T-triple and suppose there is a bounded, Borel-measurable function $\gamma: \mathbb{R} \to \mathbb{C}$ with $\gamma(h(\lambda)) \neq 0$ for ρ-a.e. $\lambda \in X$ and with $\gamma(h(\cdot))^{-1}$ bounded on each X_l[2.1]*, such that*

$$\gamma(H)\,T^{-1} \in B_2(\mathcal{H}).$$

2.1. We replaced the original condition "$\gamma(h(\cdot))^{-1}$ bounded on every set of finite ρ-measure" with "$\gamma(h(\cdot))^{-1}$ bounded on each X_l" for the following reason: if ρ is a finite measure (see [Dav95, Theorem 2.5.1]), then for the usual choice $\gamma(h) = (h - z)^{-k}$ we have that $\gamma(h(\cdot))^{-1}$ is not bounded if H is unbounded. This condition is only needed to prove that the integrals in c) are Bochner-integrable. It is therefore enough if $\gamma(h(\cdot))^{-1}$ is bounded on each X_l.

Then there exists a ρ-measurable function v: $X \to \mathcal{H}$ with $\|v(\cdot)\| \in L^2(X,\, \rho)$, such that for $u(\lambda) = \gamma(h(\lambda))^{-1}\tilde{T}v(\lambda) \in \mathcal{H}_-(T)$ we have:

a) Let $\psi \in \mathcal{H}_+(T)$. Then

$$(U\psi)(\lambda) = \langle u(\lambda), \psi\rangle \quad \text{for } \rho\text{-a.e. } \lambda;$$

b) There is some set N with $\rho(N) = 0$, such that for $\lambda \in X \setminus N$

$$\langle u(\lambda), H\psi\rangle = h(\lambda)\,\langle u(\lambda), \psi\rangle$$

holds for every $\psi \in \mathcal{E} := \{\psi \in \mathcal{H}_+(T) \cap \mathcal{D}(H)$ with $H\psi \in \mathcal{H}_+(T)\}$;

c)

$$U^*\phi = \lim_{l\to\infty} \int_{X_l} \phi(\lambda)\, u(\lambda)\, \mathrm{d}\rho(\lambda) \quad \text{for } \phi \in L^2(X, \rho),$$

and

$$\psi = \lim_{l\to\infty} \int_{X_l} (U\psi)(\lambda)\, u(\lambda)\, \mathrm{d}\rho(\lambda) \quad \text{for } \psi \in \mathcal{H}.$$

The main idea of the proof is the following: In order to find $u(\lambda)$ such that $(U\psi)(\lambda) = \langle u(\lambda), \psi\rangle$, one inserts the Hilbert-Schmidt operator $A := \gamma(H)\, T^{-1}$ and looks for $v(\lambda)$ such that $(U A\phi)(\lambda) = \langle v(\lambda), \phi\rangle$. The existence of such v is given by Theorem A.5 for the Hilbert-Schmidt operator UA: $\mathcal{H} \to L^2(X, \rho)$. Now, for $\psi = A\phi$, one (formally) has $(U\psi)(\lambda) = \langle (A^{-1})^*\, v(\lambda), \psi\rangle$ and this leads to the choice $u(\lambda) = \gamma(h(\lambda))^{-1}\, \tilde{T}v(\lambda) \in \mathcal{H}_-(T)$. This same idea was first used in [Wei87, Theorem 8.4] in the context of ordinary differential operators.

Note 2.3. A unitary operator U like the one in the hypothesis of Theorem 2.2 always exists. The multiplication version of the spectral theorem (Theorem A.2) provides the existence of a **spectral representation** $U = (U_j)$: $\mathcal{H} \to \bigoplus_{j\in\mathbb{N}} L^2(\mathbb{R}, \rho_j)$ of H; that is, the existence of finite measures ρ_j and a unitary operator U such that $U H U^* = \mathrm{Id}$ in $\bigoplus_{j\in\mathbb{N}} L^2(\mathbb{R}, \rho_j)$. We can bring this unitary equivalence in the form required in Theorem 2.2 as follows:

The direct sum of L^2-spaces $\bigoplus_{j\in\mathbb{N}} L^2(\mathbb{R}, \rho_j)$ is isometric to the space $L^2(\mathbb{R} \times \mathbb{N}, \rho)$, where the σ-finite measure ρ is defined as $\rho(A \times B) := \sum_{j\in B} \rho_j(A)$, for $A \times B \subset \mathbb{R} \times \mathbb{N}$. Therefore we can assume U: $\mathcal{H} \to L^2(\mathbb{R} \times \mathbb{N}, \rho)$. Finally, letting $h(\lambda, j) := \lambda$ for $(\lambda, j) \in \mathbb{R} \times \mathbb{N}$, it holds that $U H U^* = h$ in $L^2(\mathbb{R} \times \mathbb{N}, \rho)$.

In the situation of Theorem 2.2 above, $u(\lambda) \in \mathcal{H}_-(T)$ is called a **generalized eigenfunction** of H corresponding to the **generalized eigenvalue** $h(\lambda)$ if the set $\mathcal{E}$ of functions ψ for which b) holds is a core[2.2] for H. In this case, we say that $\psi \in \mathcal{H}$ has an **expansion in generalized eigenfunctions** $u(\lambda)$ of H, whose expression is given in c).

For the particular case where the Hilbert space is $\mathcal{H} = L^2(\mathbb{R}^d, \mathbb{C}^k)$, we can define these concepts without further reference to any self-adjoint operator T and the corresponding T-triple: Assume that $C_0^\infty(\mathbb{R}^d, \mathbb{C}^k) \subset \mathcal{D}(H)$ and $H\varphi$ has compact support for all $\varphi \in C_0^\infty(\mathbb{R}^d, \mathbb{C}^k)$. We say that $u(\lambda) \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathbb{C}^k)$ is a **generalized eigenfunction** of H corresponding to the **generalized eigenvalue** $h(\lambda)$ if

b') For all $\varphi \in C_0^\infty(\mathbb{R}^d, \mathbb{C}^k)$

$$\int \overline{u(\mathbf{x}, \lambda)}\, (H\varphi)(\mathbf{x})\, \mathrm{d}\mathbf{x} = h(\lambda) \int \overline{u(\mathbf{x}, \lambda)}\, \varphi(\mathbf{x})\, \mathrm{d}\mathbf{x}.$$

Let $u(\lambda) \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathbb{C}^k)$ be a family of generalized eigenfunctions for a.e. λ. If it holds that

a')+c) for every $\psi \in \mathcal{H}$

$$(U\psi)(\lambda) = \underset{N\to\infty}{\mathrm{l.i.m.}} \int_{|\mathbf{x}|\leqslant N} \overline{u(\mathbf{x}, \lambda)}\, \psi(\mathbf{x})\, \mathrm{d}\mathbf{x} \quad \text{for } \rho\text{-a.e. } \lambda \in X,$$

2.2. For a closed operator A, a subset $\mathcal{E} \subset \mathcal{D}(A)$ is called a **core** for A if $\overline{A \upharpoonright \mathcal{E}} = A$.

and for every $\phi \in L^2(X, \rho)$

$$U^* \phi = \lim_{l \to \infty} \int_{X_l} \phi(\lambda)\, u(\lambda)\, \mathrm{d}\rho(\lambda),$$

we say that each element in $\mathcal{H}$ has an **expansion in generalized eigenfunctions** $u(\lambda)$ of H.

The next result provides extra information about the space where the generalized eigenfunctions lie. It will be used in Theorem 3.2 for the Dirac operator to conclude some regularity of its generalized eigenfunctions.

Theorem 2.4. [PS93, Theorem 2.3] *In addition to the assumptions of Theorem 2.2 let* S *be an injective operator in* $\mathcal{H}$ *such that* $S^{-1} \in B(\mathcal{H})$ *and* $\gamma(H)\, T^{-1}\, S$ *is the restriction of a Hilbert-Schmidt operator. Then we have*

$$u(\lambda) = \gamma(h(\lambda))^{-1}\, \tilde{T}\, (S^{-1})^*\, \tilde{v}(\lambda),$$

where $\tilde{v}: X \to \mathcal{H}$ *is* ρ*-measurable,* $\|\tilde{v}(\cdot)\| \in L^2(X, \rho)$*; in particular,* $u(\lambda) \in \mathcal{R}\big(\tilde{T}\, (S^{-1})^*\big)$ *for* ρ*-a.e.* $\lambda \in X$.

2.2. Expansions for ordinary differential operators.

We now study the particular case of self-adjoint ordinary differential operators. We discussed in §2.1 how the theory for Hilbert-Schmidt operators, specifically Theorem A.5, can be useful to find expansions in generalized eigenfunctions. For ordinary differential operators it is easier to find a suitable Hilbert-Schmidt operator: the composition of the resolvent with the characteristic function of any compact interval is Hilbert-Schmidt [Wei87, Theorem 8.3][2.3]. This fact provides the existence of an expansion in generalized eigenfunctions of any ordinary differential operator [Wei87, Theorem 8.4]. If, furthermore, the resolvent kernel is known, one gets not only existence of such an expansion but it is also possible to compute it explicitly. The latter is discussed in [Wei87, Chapter 9]. In this section we summarize the results in [Wei87, Chapters 8 and 9] that we will later need for the 1-dimensional Dirac operator in §4.

We consider **differential expressions** of the form

$$\begin{aligned}\tau u(x) \;=\; & r(x)^{-1} \Bigg\{ \sum_{j=0}^{\left[\frac{n}{2}\right]} (-1)^j \big(p_j(x)\, u^{(j)}(x)\big)^{(j)} \\ & + \sum_{j=0}^{\left[\frac{n-1}{2}\right]} (-1)^j \Big[\big(q_j(x)\, u^{(j)}(x)\big)^{(j+1)} - \big(q_j^*(x)\, u^{(j+1)}(x)\big)^{(j)} \Big] \Bigg\},\end{aligned}$$

where u is a $\mathbb{C}^k$-valued function defined on (a,b), $-\infty \leqslant a < b \leqslant \infty$; the coefficients r, p_j and q_j are $k \times k$-matrix valued functions on (a,b), $r(x)$ is positive definite and the p_j are hermitian. $[\alpha]$ denotes the largest integer less than or equal to α, and so the order of the differential expression τ is n.

Let also $L^2(a,\, b;\, r)$ be the Hilbert space of $\mathbb{C}^k$-valued functions defined on $(a,\, b)$ with inner product

$$\langle u, v\rangle := \int_a^b (r(x)\, u(x), v(x))\, \mathrm{d}x,$$

where $(\cdot,\cdot)$ denotes the scalar product in $\mathbb{C}^k$.

By **self-adjoint ordinary differential operator** we mean a self-adjoint realization A of τ with domain in $L^2(a,b;r)$[2.4].

Let $z \in \mathbb{C}$. A function $u: (a,b) \to \mathbb{C}^k$ is called a **solution** of $(\tau - z)\, u = 0$ if the equation holds for almost every $x \in (a,b)$ and $u^{(j)}$ is (component-wise) absolutely continuous, for $j = 0, \ldots, n-1$. The initial value problem

$$(\tau - z)\, u = 0, \quad u^{(j)}(x_0) = u_j \quad \text{for } j = 0, \ldots, n-1$$

2.3. This does not hold in general (c.f. Note 3.4 on the 2-dimensional Dirac operator).

2.4. For $k = 2$, $n = 1$, $r(x) = \mathbb{I}$ (identity matrix), $p_0 = V\, \mathbb{I}$ and $q_0 = \frac{c}{2\,\mathrm{i}}\, \sigma_1$, τ becomes the differential expression of the 1-dimensional Dirac operator with potential V defined in §4.

has a unique solution and hence the space of all solutions of $(\tau - z)\,u = 0$ has dimension $p := n\,k$.

For a self-adjoint realization A of τ [Wei87, Theorem 8.4] proves the existence of an expansion in solutions $v_i(\cdot,\lambda)$ of $(\tau-\lambda)\,v=0$, $i=1,\ldots,p$. On the other hand, for a different choice of solutions $u_i(\cdot,\lambda)$, it is sometimes possible to compute a spectral representation which yields an expansion in terms of the $u_i(\cdot,\lambda)$. A method for this computation involving a *spectral matrix* $\rho(\lambda)$ is presented below, but we first need to discuss how a matrix-valued function $\rho(\lambda)$ defines a Hilbert space $L^2(\mathbb{R}, \mathrm{d}\,\rho)$.

Let $\rho(\lambda)$ be a non decreasing $p \times p$-matrix valued function (in the sense that, for $\lambda \geqslant \mu$, $\rho(\lambda) - \rho(\mu)$ is a positive semi-definite –and hence hermitian– matrix) such that the $\rho_{ij}(\lambda)$ are locally of bounded variation and continuous from the right. ρ defines a Hilbert space of $\mathbb{C}^p$-valued functions on $\mathbb{R}$ as follows:

Consider first $\mathbb{C}^p$-valued step functions f and g, $f(\lambda) = \sum_j \chi_{(a_j,b_j]}(\lambda)\ f_j$, $g(\lambda) = \sum_j \chi_{(a_j,b_j]}(\lambda)\,g_j$, where f_j, g_j are vectors in $\mathbb{C}^p$. We define an inner product by

$$\langle f, g\rangle_\rho := \sum_j\ ((\rho(b_j) - \rho(a_j))\ f_j, g_j) =: \int_{\mathbb{R}} (\mathrm{d}\,\rho(\lambda)\ f(\lambda), g(\lambda)),$$

and so we arrive at a pre-Hilbert space of (equivalence classes of) step functions. Its completion is a Hilbert space that we denote by $L^2(\mathbb{R}, \mathrm{d}\,\rho)$.

We can now extend our definition of **spectral representation** of A to be a unitary operator $U\colon L^2(a,b;r) \to L^2(\mathbb{R}, \mathrm{d}\,\rho)$ such that $U\,A\,U^* = \mathrm{Id}$. We finally present the method to find such a spectral representation in terms of the solutions $u_i(\cdot,\lambda)$:

Let $p := n\,k$ and assume $\{u_1(\cdot,z),\ldots,u_p(\cdot,z)\}$ is a family of p linearly independent solutions of $(\tau-z)\,u=0$ which are entire functions of z. For each $z\in\rho(A)$ the resolvent $(A-z)^{-1}$ is an integral kernel operator [Wei87, §7] and there exist uniquely determined functions $m_{ij}^+, m_{ij}^-\colon \rho(A)\to\mathbb{C}$ such that the integral kernel is

$$R(x,y,z) \;=\; \begin{cases} \sum_{i,j=1}^p m_{ij}^+(z)\,u_i(x,z)\,\overline{u_j(y,\bar z)} & \text{for } y \leqslant x,\\ \sum_{i,j=1}^p m_{ij}^-(z)\,u_i(x,z)\,\overline{u_j(y,\bar z)} & \text{for } y > x.\end{cases}$$

Let the **spectral matrix** $\rho(\lambda)$ be defined by

$$\rho_{ij}(\lambda) = \frac{1}{2\,\pi\,\mathrm{i}}\lim_{\delta\to 0_+}\lim_{\varepsilon\to 0_+}\int_\delta^{\lambda+\delta} \left(m_{ij}^{\pm}(s+\mathrm{i}\,\varepsilon) - \overline{m_{ji}^{\mp}(s+\mathrm{i}\,\varepsilon)}\right)\mathrm{d}s. \tag{2.1}$$

We have

Theorem 2.5. *Let A be a self-adjoint realization of τ, let $\{u_1,\ldots,u_p\}$ and ρ be as above. Then $F\colon L^2(a,b;r)\to L^2(\mathbb{R},\mathrm{d}\,\rho)$*

$$(F_i\,\psi)(\lambda) \;=\; \underset{\substack{\alpha\to a_+\\ \beta\to b_-}}{\mathrm{l.i.m.}} \int_\alpha^\beta (r(x)\,u_i(x,\lambda), \psi(x))\,\mathrm{d}x \qquad i=1,\ldots,p$$

is a spectral representation of A. Its inverse is given by

$$(F^{-1}\,\phi)(x) \;=\; \underset{N\to\infty}{\mathrm{l.i.m.}} \sum_{i,j=1}^p \int_{-N}^N u_j(x,\lambda)\,\phi_i(\lambda)\,\mathrm{d}\,\rho_{ji}(\lambda).$$

Theorem 2.5 is the combination of [Wei87, Theorem 8.7] and [Wei87, Corollary 9.6].

3. Generalized eigenfunctions of the 2-D massless Dirac operator

In this section we apply the results on BGK expansions stated in §2.1 to the 2-dimensional massless Dirac operator with electromagnetic potentials within a large class of functions. In §3.2 we prove that the generalized eigenfunctions of the 2-dimensional Dirac operator lie in certain weighted Sobolev spaces. For this purpose we find appropriated Hilbert-Schmidt operators involving a power of the resolvent and the multiplication by a weight $\langle \mathbf{x}\rangle^{-s}$. This is done by using a *weighted resolvent identity* (Lemma 3.3), which turns out to be very useful in this context.

A direct consequence of the BGK expansions (see Theorem 2.2) is that every point in the spectrum can be approximated by generalized eigenvalues. A kind of converse of this statement also holds. We prove this relationship between the spectrum and the generalized eigenvalues of the 2-dimensional Dirac operator in §3.3.

The questions we discuss here were also studied in Stolz's Doctoral Thesis for the 3-dimensional Dirac operator [Sto89, §6]. Nevertheless, this section has been written in a completely independent way, since we were unaware of the existence of Stolz's results at the time we were working on it.

3.1. Definition of the 2-D operator.

Let us first describe the Dirac operators formally without specifying their domains. The domains and self-adjointness are discussed in Lemma 3.1 below.

The 2-dimensional massless Dirac operator with a magnetic field B on $\mathcal{H}:=L^2(\mathbb{R}^2,\mathbb{C}^2)$ has the form

$$\tilde{H}_{\boldsymbol{A}}:=\boldsymbol{\sigma}\cdot(\boldsymbol{p}-\boldsymbol{A}),$$

where the magnetic vector potential $\boldsymbol{A}:\mathbb{R}^2\to\mathbb{R}^2$ satisfies $B=\mathrm{rot}\boldsymbol{A}:=\partial_1 A_2-\partial_2 A_1$, $\boldsymbol{p}:=-\mathrm{i}\,\nabla$ and $\boldsymbol{\sigma}=(\sigma_1,\sigma_2)$ with

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

For an electric potential $V:\mathbb{R}^2\to\mathbb{R}$, we define

$$\tilde{H}:=\tilde{H}_{\boldsymbol{A}}+V.$$

We also introduce the notation for the free Dirac operator

$$\tilde{H}_0:=\boldsymbol{\sigma}\cdot\boldsymbol{p}.$$

Lemma 3.1. *For the $\tilde{H}_0$, $\tilde{H}_{\boldsymbol{A}}$ and $\tilde{H}$ formally defined above the following statements hold:*

a) *$\tilde{H}_0$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^2,\mathbb{C}^2)$.*

b) *For $\boldsymbol{A}\in L^p_{\mathrm{loc}}(\mathbb{R}^2,\mathbb{R}^2)$ and $V\in L^p_{\mathrm{loc}}(\mathbb{R}^2,\mathbb{R})$ with $2<p\leqslant\infty$, $\tilde{H}_{\boldsymbol{A}}$ and $\tilde{H}$ are essentially self-adjoint on $C_0^\infty(\mathbb{R}^2,\mathbb{C}^2)$.*

c) *For $B\in L^q_{\mathrm{loc}}(\mathbb{R}^2,\mathbb{R})$ with $1<q<\infty$, there exists $\boldsymbol{A}\in L^p_{\mathrm{loc}}(\mathbb{R}^2,\mathbb{R}^2)$ with $2<p\leqslant\infty$ and $B=\mathrm{rot}\,\boldsymbol{A}$.*

For the proofs of b) resp. c) we follow [KS12, §3.1 resp. Remark 8].

Proof. a) First note that $\tilde{H}_0$ is unitarily equivalent to the multiplication operator $\boldsymbol{\sigma}\cdot\boldsymbol{p}$ in the Fourier space, where $\boldsymbol{p}$ also denotes the Fourier variable. This multiplication operator is self-adjoint in its domain $\{\hat{\psi}:(1+\boldsymbol{\sigma}\cdot\boldsymbol{p})\,\hat{\psi}(\boldsymbol{p})\in L^2(\mathbb{R}^2,\mathbb{C}^2)\}=\{\hat{\psi}:(1+\boldsymbol{p})\,\hat{\psi}(\boldsymbol{p})\in L^2(\mathbb{R}^2,\mathbb{C}^2)\}$, which is the Fourier transformed of the Sobolev space $H^1(\mathbb{R}^2,\mathbb{C}^2)$. Therefore the operator $\tilde{H}_0$ defined on $H^1(\mathbb{R}^2,\mathbb{C}^2)$ is self-adjoint. We denote this operator by H_0.

We now only need to show that the closure in $\mathcal{H}\times\mathcal{H}$ of the graph of $\tilde{H}_0$ defined on C_0^∞ is the graph of the self-adjoint operator H_0, that is,

$$\overline{\{(\varphi,\tilde{H}_0\,\varphi):\varphi\in C_0^\infty(\mathbb{R}^2,\mathbb{C}^2)\}}=\{(\psi,H_0\,\psi):\psi\in H^1(\mathbb{R}^2,\mathbb{C}^2)\}.$$

Indeed, the right to left inclusion holds because $C_0^\infty(\mathbb{R}^2,\mathbb{C}^2)$ is dense in $H^1(\mathbb{R}^2,\mathbb{C}^2)$ and $\|\cdot\|_{H^1}^2 := \|\cdot\|^2+\|\partial_1\cdot\|^2+\|\partial_2\cdot\|^2=\|\cdot\|^2+\big\|\tilde{H}_0\cdot\big\|^2$, so given $\psi\in H^1(\mathbb{R}^2,\mathbb{C}^2)$ there exists a sequence $\varphi_n\in C_0^\infty(\mathbb{R}^2,\mathbb{C}^2)$ such that $\big(\varphi_n,\tilde{H}_0\,\varphi_n\big)\to(\psi,H_0\,\psi)$ in $\mathcal{H}\times\mathcal{H}$. The left to right inclusion follows from

$$\varphi_n\in C_0^\infty(\mathbb{R}^2,\mathbb{C}^2)\quad\text{such that}\quad\begin{cases}\varphi_n\to\psi\in\mathcal{H}\\ \tilde{H}_0\,\varphi_n\to\phi\in\mathcal{H}\end{cases}\Rightarrow\quad\psi\in H^1(\mathbb{R}^2,\mathbb{C}^2)\quad\text{and}\quad\tilde{H}_0\,\psi=\phi.$$

b) We prove this only for $\tilde{H}$ since $\tilde{H}_{\boldsymbol{A}}$ is the particular case for $V=0$.

[Che77, Theorem 2.1] implies that the essential self-adjointness of $\tilde{H}$ depends only on the local behaviour of $\boldsymbol{A}$ and V. Consequently, we only need study the self-adjointness of the operators $\tilde{H}_\Omega$ defined on C_0^∞ by

$$\tilde{H}_\Omega:=\boldsymbol{\sigma}\cdot(\boldsymbol{p}-\chi(\Omega)\,\boldsymbol{A})+\chi(\Omega)\,V,$$

where $\Omega\subset\mathbb{R}^2$ is a bounded domain.

If $2<p<\infty$ and $z\in\mathbb{C}\backslash\mathbb{R}$, the function $g(\mathbf{x}):=(\boldsymbol{\sigma}\cdot\mathbf{x}-z)^{-1}$ is in $L^p(\mathbb{R}^2,\mathbb{C}^4)$. By [Sim10, Theorem 4.1], the operator $f(\mathbf{x})\;g(-\mathrm{i}\;\nabla)=f(\mathbf{x})\;R_0(z)$ is compact for any $f\in L^p(\mathbb{R}^2,\,\mathbb{C}^4)$. Hence, $f=\chi(\Omega)\,V\,\mathbb{I}-\boldsymbol{\sigma}\cdot\chi(\Omega)\,\boldsymbol{A}\in L^p$ is a relatively compact perturbation of H_0, and therefore $H_0+f=\tilde{H}_\Omega$ is essentially self-adjoint on C_0^∞.

If $p=\infty$, the operator $\chi(\Omega)\,V-\boldsymbol{\sigma}\cdot\chi(\Omega)\,\boldsymbol{A}$ is H_0-bounded with relative bound 0:

$$\|(\chi(\Omega)\,V-\boldsymbol{\sigma}\cdot\chi(\Omega)\,\boldsymbol{A})\,\psi\|_2\leqslant2\,\|\chi(\Omega)\,(V-\boldsymbol{A})\|_\infty\|\psi\|_2$$

and the Kato-Rellich Theorem [RS75, Theorem X.12] implies that $\tilde{H}_\Omega$ is essentially self-adjoint on C_0^∞.

c) Let h be a solution of $\Delta h=B$. For $\Omega\subset\mathbb{R}^2$ bounded, a solution of $\Delta h=B$ on Ω is given by the Newtonian potential h_N of B

$$h_N(\mathbf{x}):=\int_\Omega\Gamma(\mathbf{x}-\mathbf{y})\,B(\mathbf{y})\,\mathrm{d}\mathbf{y},$$

where Γ is the fundamental solution of the Laplace equation. By [GT01, Theorem 9.9] $h_N\in W^{2,q}(\Omega)$ and $\Delta h_N=B$ a.e in Ω. Then, h_N-h is harmonic on Ω and hence $C^\infty(\Omega)$, which implies that $h\in W_{\mathrm{loc}}^{2,q}(\mathbb{R}^2)$. $\boldsymbol{A}:=(-\partial_2h,\partial_1h)$ satisfies $B=\mathrm{rot}\,\boldsymbol{A}$ and $\boldsymbol{A}\in W_{\mathrm{loc}}^{1,q}(\mathbb{R}^2,\mathbb{R}^2)$. The Sobolev inequalities (see, for instance, [LL01, Theorem 8.8]) lead to the conclusion that $\boldsymbol{A}\in L_{\mathrm{loc}}^p(\mathbb{R}^2,\,\mathbb{R}^2)$ for some $2<p<\infty$ if $q\in(1,2]$, or $\boldsymbol{A}\in L_{\mathrm{loc}}^\infty(\mathbb{R}^2,\mathbb{R}^2)$ if $q>2$. □

Throughout the rest of Section 3 $\mathcal{H}$ will denote the Hilbert space $L^2(\mathbb{R}^2,\,\mathbb{C}^2)$, $\boldsymbol{A}$ and V will denote functions in $L_{\mathrm{loc}}^p(\mathbb{R}^2,\mathbb{R}^2)$ resp. $L_{\mathrm{loc}}^p(\mathbb{R}^2,\mathbb{R})$ for $p>2$, and $H_0,H_{\boldsymbol{A}},H$ the corresponding self-adjoint extensions in $\mathcal{H}$ of the operators $\tilde{H}_0,\tilde{H}_{\boldsymbol{A}},\tilde{H}$ defined on $C_0^\infty(\mathbb{R}^2,\mathbb{C}^2)$.

3.2. Properties of the generalized eigenfunctions.

The main result of this section is

Theorem 3.2. *Let H be the two-dimensional Dirac operator defined in §3.1 and assume $\boldsymbol{A}\in L_{-s}^\infty(\mathbb{R}^2,\mathbb{R}^2)$, $V\in L_{-s}^\infty(\mathbb{R}^2,\mathbb{R})$ for some $s\geqslant0$. Then, for any $k>\frac{1}{2}$, there exist families $u_1(\lambda)\in L_{-2(s+k)}^2(\mathbb{R}^2,\mathbb{C}^2)$ and $u_2(\lambda)\in H_{-(3s+2k)}^1(\mathbb{R}^2,\mathbb{C}^2)$ of generalized eigenfunctions of H, each of which expands any $\psi\in\mathcal{H}=L^2(\mathbb{R}^2,\mathbb{C}^2)$.*

We will prove this at the end of the section applying Theorem 2.2 and Theorem 2.4, but we first need to find suitable Hilbert-Schmidt operators. We split this problem in several lemmas below. The first of these proves what we called *weighted resolvent identity*, a generalization of the usual resolvent identity[3.1] including a weight, which will be very useful for finding the Hilbert-Schmidt operators.

3.1. $A^{-1}-B^{-1}=B^{-1}\,(B-A)\,A^{-1}$ holds on $\mathcal{H}$ for invertible operators A and B with bounded inverse and such that $\mathcal{D}(A)\subset\mathcal{D}(B)$.

Lemma 3.3. (**Weighted resolvent identity**)[3.2] *Assume* $\boldsymbol{A}\in L^{\infty}_{-s}(\mathbb{R}^2,\mathbb{R}^2), V\in L^{\infty}_{-s}(\mathbb{R}^2,\mathbb{R})$ *for some* $s\geqslant 0$ *and let* $z\in\mathbb{C}$ *with* $|\mathrm{Im}\, z|>2\, s$*. Then the following identity of operators on* $\mathcal{H}$ *holds:*

$$R(z)\,\langle\mathbf{x}\rangle^{-s}=R_0(z)\,\langle\mathbf{x}\rangle^{-s}+R_0(z)\,\langle\mathbf{x}\rangle^{-s}\,(H_0-H)\,R(z)\,D^{-1}, \tag{3.1}$$

where

$$D:=\left(1+s\,\frac{\mathrm{i}\,\boldsymbol{\sigma}\cdot\mathbf{x}}{\langle\mathbf{x}\rangle^2}\,R(z)\right).$$

Note that for $s=0$ this is the usual resolvent identity for H and H_0.

Proof. Let $\varphi\in C_0^{\infty}(\mathbb{R}^2,\mathbb{C}^2)$, then

$$\begin{aligned} R(z)\,\langle\mathbf{x}\rangle^{-s}\,(H-z)\varphi &= \langle\mathbf{x}\rangle^{-s}\,\varphi+R(z)\,[\langle\mathbf{x}\rangle^{-s},H]\,\varphi \\ &= \langle\mathbf{x}\rangle^{-s}\,\varphi+R(z)\,(\mathrm{i}\,\boldsymbol{\sigma}\cdot\nabla\,\langle\mathbf{x}\rangle^{-s})\,\varphi. \end{aligned} \tag{3.2}$$

Similarly we have

$$\begin{aligned} \langle\mathbf{x}\rangle^{-s}\,\varphi &= R_0(z)\,(H_0-z)\,\langle\mathbf{x}\rangle^{-s}\,\varphi \\ &= R_0(z)\,\langle\mathbf{x}\rangle^{-s}\,(H_0-z)\,\varphi+R_0(z)\,[H_0,\langle\mathbf{x}\rangle^{-s}]\,\varphi \\ &= R_0(z)\,\langle\mathbf{x}\rangle^{-s}\,(H_0-z)\,\varphi-R_0(z)\,(\mathrm{i}\,\boldsymbol{\sigma}\cdot\nabla\,\langle\mathbf{x}\rangle^{-s})\,\varphi \\ &= R_0(z)\,\langle\mathbf{x}\rangle^{-s}\,(H-z)\,\varphi+R_0(z)\,\langle\mathbf{x}\rangle^{-s}\,(H_0-H)\,\varphi-R_0(z)\,(\mathrm{i}\,\boldsymbol{\sigma}\cdot\nabla\,\langle\mathbf{x}\rangle^{-s})\,\varphi. \end{aligned} \tag{3.3}$$

(3.2) and (3.3) yield

$$\begin{aligned} R(z)\,\langle\mathbf{x}\rangle^{-s}\,(H-z)\varphi &= R_0(z)\,\langle\mathbf{x}\rangle^{-s}\,(H-z)\,\varphi+R_0(z)\,\langle\mathbf{x}\rangle^{-s}\,(H_0-H)\,\varphi \\ &\quad +(R(z)-R_0(z))\,(\mathrm{i}\,\boldsymbol{\sigma}\cdot\nabla\,\langle\mathbf{x}\rangle^{-s})\,\varphi. \end{aligned} \tag{3.4}$$

We can extend the identity (3.4) to any $\varphi\in\mathcal{D}(H)$, since H is the closure of its restriction to $C_0^{\infty}(\mathbb{R}^2,\mathbb{C}^2)$. Indeed, this implies that for any $\varphi\in\mathcal{D}(H)$ there exists a sequence $(\varphi_n)\subset C_0^{\infty}(\mathbb{R}^2,\mathbb{C}^2)$ with $\varphi_n\to\varphi$ and $H\varphi_n\to H\varphi$ in $\mathcal{H}$. From $\boldsymbol{A}\in L^{\infty}_{-s}(\mathbb{R}^2,\,\mathbb{R}^2)$, $V\in L^{\infty}_{-s}(\mathbb{R}^2,\,\mathbb{R})$ follows that $\langle\mathbf{x}\rangle^{-s}\,(H_0-H)=\langle\mathbf{x}\rangle^{-s}\,(\boldsymbol{\sigma}\cdot\boldsymbol{A}-V)$ is a bounded operator. Since $\langle\mathbf{x}\rangle^{-s}$ and $\nabla\,\langle\mathbf{x}\rangle^{-s}$ are also bounded, we have

$$\langle\mathbf{x}\rangle^{-s}\,(H-z)\,\varphi_n\to\langle\mathbf{x}\rangle^{-s}\,(H-z)\,\varphi,$$

$$\langle\mathbf{x}\rangle^{-s}\,(H_0-H)\,\varphi_n\to\langle\mathbf{x}\rangle^{-s}\,(H_0-H)\,\varphi$$

and

$$\nabla\,\langle\mathbf{x}\rangle^{-s}\,\varphi_n\to\nabla\,\langle\mathbf{x}\rangle^{-s}\,\varphi$$

in $\mathcal{H}$. Hence, by taking limits on both sides, we obtain the identity for any $\varphi\in\mathcal{D}(H)$. We can also write (3.4) as

$$\begin{aligned} R(z)\,\langle\mathbf{x}\rangle^{-s}\,(H-z)\varphi &= R_0(z)\,\langle\mathbf{x}\rangle^{-s}\,(H-z)\,\varphi \\ &\quad +R_0(z)\,\langle\mathbf{x}\rangle^{-s}\,(H_0-H)\,R(z)(H-z)\,\varphi \\ &\quad +(R(z)-R_0(z))\,(\mathrm{i}\,\boldsymbol{\sigma}\cdot\nabla\,\langle\mathbf{x}\rangle^{-s})\,R(z)\,(H-z)\,\varphi, \end{aligned} \tag{3.5}$$

where we just replaced φ by $R(z)\,(H-z)\,\varphi$ in the two last terms. Since $z\notin\sigma(H)\subset\mathbb{R}$, in particular we have $\mathrm{Ran}\,(H-z)=\mathcal{H}$ and (3.5) becomes

$$\begin{aligned} R(z)\,\langle\mathbf{x}\rangle^{-s}\,\psi &= R_0(z)\,\langle\mathbf{x}\rangle^{-s}\,\psi+R_0(z)\,\langle\mathbf{x}\rangle^{-s}\,(H_0-H)\,R(z)\,\psi \\ &\quad +(R(z)-R_0(z))\,(\mathrm{i}\,\boldsymbol{\sigma}\cdot\nabla\,\langle\mathbf{x}\rangle^{-s})\,R(z)\,\psi, \end{aligned} \tag{3.6}$$

for all $\psi\in\mathcal{H}$. Writing $\mathrm{i}\,\boldsymbol{\sigma}\cdot\nabla\,\langle\mathbf{x}\rangle^{-s}$ in (3.6) as $\langle\mathbf{x}\rangle^{-s}\,\langle\mathbf{x}\rangle^{s}\,\mathrm{i}\,\boldsymbol{\sigma}\cdot\nabla\,\langle\mathbf{x}\rangle^{-s}=-\langle\mathbf{x}\rangle^{-s}\,s\,\dfrac{\mathrm{i}\,\boldsymbol{\sigma}\cdot\mathbf{x}}{\langle\mathbf{x}\rangle^2}$ and grouping terms we get

$$(R(z)-R_0(z))\,\langle\mathbf{x}\rangle^{-s}\left(1+s\,\frac{\mathrm{i}\,\boldsymbol{\sigma}\cdot\mathbf{x}}{\langle\mathbf{x}\rangle^2}\,R(z)\right)=R_0(z)\,\langle\mathbf{x}\rangle^{-s}\,(H_0-H)\,R(z), \tag{3.7}$$

3.2. We owe Prof. E. Stockmeyer the idea of this identity.

as an identity of operators on $\mathcal{H}$. Finally, since

$$\left\| s\,\frac{\mathrm{i}\,\boldsymbol{\sigma}\cdot\mathbf{x}}{\langle\mathbf{x}\rangle^2}\,R(z)\right\| \leqslant 2\,s\left\|\frac{\mathbf{x}}{\langle\mathbf{x}\rangle^2}\right\|_\infty \|R(z)\| \leqslant 2\,s\,\|R(z)\| \leqslant 2\,s\,\frac{1}{|\mathrm{Im}\,z|},$$

which is less than 1 by hypothesis, we conclude that $D := \left(1 + s\,\frac{\mathrm{i}\,\boldsymbol{\sigma}\cdot\mathbf{x}}{\langle\mathbf{x}\rangle^2}\,R(z)\right)$ is an invertible operator. Right-composition with D^{-1} on both sides of (3.7) yields (3.1). □

Note 3.4. If $R_0(z)\,\langle\mathbf{x}\rangle^{-k}$ were a Hilbert-Schmidt operator for some $z\in\mathbb{C}\backslash\mathbb{R}$ and $k\geqslant 0$, we could use Lemma 3.3 with $\langle\mathbf{x}\rangle^{-(s+k)}$ to prove that $R(z)\,\langle\mathbf{x}\rangle^{-(s+k)}$ is Hilbert-Schmidt:

$$\begin{aligned} R(z)\,\langle\mathbf{x}\rangle^{-(s+k)} &= R_0(z)\,\langle\mathbf{x}\rangle^{-(s+k)} + R_0(z)\,\langle\mathbf{x}\rangle^{-(s+k)}\,(H_0 - H)\,R(z)\,D^{-1} \\ &= R_0(z)\,\langle\mathbf{x}\rangle^{-k}(\langle\mathbf{x}\rangle^{-s} + \langle\mathbf{x}\rangle^{-s}\,(H_0 - H)\,R(z)\,D^{-1}), \end{aligned}$$

and this is the composition of a Hilbert-Schmidt operator and a bounded operator (since $\langle\mathbf{x}\rangle^{-s}\,(H_0 - H)$ is bounded). But it is not true that $R_0(z)\,\langle\mathbf{x}\rangle^{-k}$ is Hilbert-Schmidt for some k. In fact, it holds

$R_0(z)\,f$ is not Hilbert-Schmidt for any choice of $z\in\mathbb{C}\backslash\mathbb{R}$ and $f\in L^2(\mathbb{R}^2,\mathbb{C})$.

Indeed, we can first write the resolvent as

$$R_0(z) = (H_0 - z)^{-1} = (H_0 + z)\,(H_0^2 - z^2)^{-1} = (H_0 + z)\,(-\Delta - z^2)^{-1}. \tag{3.8}$$

On the other hand, for any $\psi\in\mathcal{H}$,

$$\begin{aligned} (-\Delta - z^2)^{-1}\,f\psi &= \mathcal{F}^{-1}((\mathbf{p}^2 - z^2)^{-1}\,\mathcal{F}(f\psi)(\mathbf{p})) \qquad (3.9)\\ &= h*(f\psi), \end{aligned}$$

where $h := (2\,\pi)^{-1}\,\mathcal{F}^{-1}((\boldsymbol{p}^2 - z^2)^{-1})$. Using (3.8) and (3.9) we can write the considered operator as an integral operator,

$$\begin{aligned} (R_0(z)\,f\psi)(\mathbf{x}) &= (H_0 + z)\int h(\mathbf{x}-\mathbf{y})\,f(\mathbf{y})\,\psi(\mathbf{y})\,\mathrm{d}\mathbf{y} \\ &= \int\,(-\mathrm{i}\,\boldsymbol{\sigma}\,\nabla_{\mathbf{x}} + z)\,h(\mathbf{x}-\mathbf{y})\,f(\mathbf{y})\,\psi(\mathbf{y})\,\mathrm{d}\mathbf{y} \\ &= \int k(\mathbf{x},\mathbf{y})\,\psi(\mathbf{y})\,\mathrm{d}\mathbf{y} \quad \text{for all } \psi\in\mathcal{H} \text{ and a.e. } \mathbf{x}\in\mathbb{R}^2, \end{aligned}$$

with integral kernel $k(\mathbf{x},\mathbf{y}) := (-\mathrm{i}\,\boldsymbol{\sigma}\,\nabla_{\mathbf{x}} + z)\,h(\mathbf{x}-\mathbf{y})\,f(\mathbf{y})$. Now this operator is Hilbert-Schmidt if and only if the kernel is in $L^2(\mathbb{R}^2\times\mathbb{R}^2, \mathrm{d}\mathbf{x}\otimes\mathrm{d}\mathbf{y})$ (Theorem A.4), and the latter happens if and only if both f and $(-\mathrm{i}\,\boldsymbol{\sigma}\,\nabla + z)\,h$ are in L^2. Using Plancherel's identity we conclude that

$$\|(-\mathrm{i}\,\boldsymbol{\sigma}\,\nabla + z)\,h\|_2 = \|\mathcal{F}\,(-\mathrm{i}\,\boldsymbol{\sigma}\,\nabla + z)\,h\|_2 = C\left\|\frac{\boldsymbol{p} + z}{\boldsymbol{p}^2 - z^2}\right\|_2 = \infty,$$

since $\frac{\boldsymbol{p}+z}{\boldsymbol{p}^2 - z^2}\notin L^2(\mathbb{R}^2)$.

Following this same idea, it is now easy to check that squaring the resolvent and adding a weight one obtains a Hilbert-Schmidt operator.

Lemma 3.5. *Let $z, w\in\mathbb{C}\backslash\mathbb{R}$. Then $R_0(w)\,R_0(z)\,\langle\mathbf{x}\rangle^{-s}$ is Hilbert-Schmidt for $s > 1$.*

Proof. We can assume $z = w$. The general case follows using the resolvent identity, since we can write $R_0(w)\,R_0(z)\,\langle\mathbf{x}\rangle^{-s}$ as the composition of $R_0(z)^2\,\langle\mathbf{x}\rangle^{-s}$ with a bounded operator:

$$\begin{aligned} R_0(w)\,R_0(z)\,\langle\mathbf{x}\rangle^{-s} &= R_0(z)^2\,\langle\mathbf{x}\rangle^{-s} + (R_0(w) - R_0(z))\,R_0(z)\,\langle\mathbf{x}\rangle^{-s} \\ &= R_0(z)^2\,\langle\mathbf{x}\rangle^{-s} + (z - w)\,R_0(w)\,R_0(z)^2\,\langle\mathbf{x}\rangle^{-s} \\ &= (1 + (z - w)\,R_0(w))\,R_0(z)^2\,\langle\mathbf{x}\rangle^{-s}. \end{aligned}$$

We now prove that $R_0(z)^2\,\langle\mathbf{x}\rangle^{-s}$ is Hilbert-Schmidt with the same argument as in Note 3.4. From (3.8), and since (H_0+z) and $(-\Delta-z^2)^{-1}=(H_0^2-z^2)^{-1}$ commute, we have

$$R_0(z)^2=(H_0+z)^2\,(-\Delta-z^2)^{-2}. \tag{3.10}$$

Now, for any $\psi\in\mathcal{H}$,

$$\begin{aligned}(-\Delta-z^2)^{-2}\,\langle\mathbf{x}\rangle^{-s}\,\psi &= \mathcal{F}^{-1}((\mathbf{p}^2-z^2)^{-2}\,\mathcal{F}(\langle\mathbf{x}\rangle^{-s}\,\psi)(\mathbf{p}))\\ &= g*(\langle\mathbf{x}\rangle^{-s}\,\psi),\end{aligned} \tag{3.11}$$

where $g:=(2\,\pi)^{-1}\,\mathcal{F}^{-1}((\boldsymbol{p}^2-z^2)^{-2})$. As before, we use (3.10) and (3.11) to write the operator in an integral form

$$\begin{aligned}(R_0(z)^2\,\langle\mathbf{x}\rangle^{-s}\,\psi)(\mathbf{x}) &= (H_0+z)^2\int g(\mathbf{x}-\mathbf{y})\,\langle\mathbf{y}\rangle^{-s}\,\psi(\mathbf{y})\,\mathrm{d}\mathbf{y}\\ &= \int K(\mathbf{x},\mathbf{y})\,\psi(\mathbf{y})\,\mathrm{d}\mathbf{y}\quad\text{for all } \psi\in\mathcal{H} \text{ and a.e. } \mathbf{x}\in\mathbb{R}^2,\end{aligned}$$

where $K(\mathbf{x},\mathbf{y}):=(-\Delta_{\mathbf{x}}-2\,\mathrm{i}\,z\boldsymbol{\sigma}\cdot\nabla_{\mathbf{x}}+z^2)\,g(\mathbf{x}-\mathbf{y})\,\langle\mathbf{y}\rangle^{-s}$. In this case, we do have that the integral kernel K is in $L^2(\mathbb{R}^2\times\mathbb{R}^2,\mathrm{d}\mathbf{x}\otimes\mathrm{d}\mathbf{y})$:

$$\begin{aligned}\|K(\mathbf{x},\mathbf{y})\|^2_{L^2(\mathbb{R}^2\times\mathbb{R}^2)} &= \int|(-\Delta_{\mathbf{x}}-2\,\mathrm{i}\,z\boldsymbol{\sigma}\cdot\nabla_{\mathbf{x}}+z^2)\,g(\mathbf{x}-\mathbf{y})|^2\,\langle\mathbf{y}\rangle^{-2s}\,\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y}\\ &= \int|(-\Delta_{\mathbf{x}}-2\,\mathrm{i}\,z\boldsymbol{\sigma}\cdot\nabla_{\mathbf{x}}+z^2)\,g(\mathbf{x})|^2\,\mathrm{d}\mathbf{x}\int\langle\mathbf{y}\rangle^{-2s}\,\mathrm{d}\mathbf{y}\\ &= \int\left|\frac{\mathbf{p}^2+2\,z\,\boldsymbol{\sigma}\cdot\mathbf{p}+z^2}{(\mathbf{p}^2-z^2)^2}\right|^2\mathrm{d}\mathbf{p}\int\langle\mathbf{y}\rangle^{-2s}\,\mathrm{d}\mathbf{y}<\infty,\end{aligned}$$

and therefore the considered operator is Hilbert-Schmidt. □

Now that we know $R_0(z)^2\,\langle\mathbf{x}\rangle^{-s}$ is Hilbert-Schmidt for $s>1$, we want to find a relation which allows us to prove that $R(w)^2\,\langle\mathbf{x}\rangle^{-k}$ is Hilbert-Schmidt for some $w\notin\mathbb{R}$ and $k\geqslant 0$. This will be achieved with the following lemma together with the weighted resolvent identity.

Lemma 3.6. *Let $s\geqslant 0$ and $z\in\mathbb{C}$ with $|\mathrm{Im}\,z|>4\,s$. Then*

$$R_j(z)^2\,\langle\mathbf{x}\rangle^{-2s}\in B_2(\mathcal{H})\quad\textit{if and only if}\quad\langle\mathbf{x}\rangle^{-s}\,R_j(\bar z\,)\,R_j(z)\,\langle\mathbf{x}\rangle^{-s}\in B_2(\mathcal{H}),$$

for $j\in\{0,1\}$[3.3].

Proof. We prove this in two steps. First, we show

$$R_j(z)\,\langle\mathbf{x}\rangle^{-2s}\,R_j(z)\in B_2(\mathcal{H})\quad\textit{if and only if}\quad\langle\mathbf{x}\rangle^{-s}\,R_j(\bar z\,)\,R_j(z)\,\langle\mathbf{x}\rangle^{-s}\in B_2(\mathcal{H}) \tag{3.12}$$

and we finish with

$$R_j(z)^2\,\langle\mathbf{x}\rangle^{-2s}\in B_2(\mathcal{H})\quad\textit{if and only if}\quad R_j(z)\,\langle\mathbf{x}\rangle^{-2s}\,R_j(z)\in B_2(\mathcal{H}), \tag{3.13}$$

which together yield the statement of the theorem. For (3.12) first notice that $R_j(z)\,\langle\mathbf{x}\rangle^{-2s}\,R_j(z)$ being Hilbert-Schmidt is equivalent to $R_j(z)\,\langle\mathbf{x}\rangle^{-2s}\,R_j(\bar z\,)$ being Hilbert-Schmidt:

$$\begin{aligned}R_j(z)\,\langle\mathbf{x}\rangle^{-2s}\,R_j(\bar z\,) &= R_j(z)\,\langle\mathbf{x}\rangle^{-2s}\,R_j(z)+R_j(z)\,\langle\mathbf{x}\rangle^{-2s}\,(R_j(\bar z\,)-R_j(z))\\ &= R_j(z)\,\langle\mathbf{x}\rangle^{-2s}\,R_j(z)+(z-\bar z\,)\,R_j(z)\,\langle\mathbf{x}\rangle^{-2s}\,R_j(\bar z\,)\,R_j(z)\\ &= R_j(z)\,\langle\mathbf{x}\rangle^{-2s}\,R_j(z)\,(1+2\,\mathrm{Im}\,z\,R_j(\bar z\,)),\end{aligned}$$

where we used the resolvent identity for the second equality. Since $(1+2\,\mathrm{Im}\,z\,R_j(\bar z\,))$ is a bounded operator, if $R_j(z)\,\langle\mathbf{x}\rangle^{-2s}\,R_j(z)$ is Hilbert-Schmidt then so is $R_j(z)\,\langle\mathbf{x}\rangle^{-2s}\,R_j(\bar z\,)$. The converse is proved analogously.

Now call $A:=R_j(z)\,\langle\mathbf{x}\rangle^{-s}$. A is a bounded operator on $\mathcal{H}$ and what remains to prove is

$$A\,A^*\ \textit{is Hilbert-Schmidt if and only if}\ A^*\,A\ \textit{is Hilbert-Schmidt}. \tag{3.14}$$

3.3. This result holds for both H_0 and H. We write an index $j\in\{0,1\}$ to prove it for both cases: $j=0$ refers to the free case, while $j=1$ refers (only in this lemma) to the case with external potentials.

There exists a partial isometry $U\colon (\ker A)^{\perp} \to (\ker A^*)^{\perp}$ such that $A = U\,|A|$ (this is known as the *polar decomposition* of A, see [RS80, Theorem VI.10]). In our case U is a total isometry –a unitary operator–, since $\ker R_j(z) = \{0\}$ and $\langle \mathbf{x} \rangle^{-s} \not\equiv 0$, which means that both $\ker A$ and $\ker A^*$ are trivial. We have

$$A\,A^* = U\,|A|\,|A|\,U^{-1} = U\,A^* A\,U^{-1}. \tag{3.15}$$

Since unitarily equivalent operators have the same trace and, from (3.15), the operators $(A\,A^*)^2$ and $(A^*\,A)^2$ are unitarily equivalent, we conclude (3.14)[3.4].

For the proof of (3.13), let $\varphi \in \mathcal{D}(H_j)$. First note that also $\langle \mathbf{x} \rangle^{-s}\,\varphi \in \mathcal{D}(H_j)$:

$$\begin{aligned} \|H_j\,\langle \mathbf{x} \rangle^{-s}\,\varphi\| &= \|\langle \mathbf{x} \rangle^{-s}\,H_j\,\varphi - (\mathrm{i}\,\boldsymbol{\sigma}\,\nabla\,\langle \mathbf{x} \rangle^{-s})\,\varphi\| \\ &\leqslant \|\langle \mathbf{x} \rangle^{-s}\|_\infty\,\|H_j\,\varphi\| + 2\,\|\nabla\,\langle \mathbf{x} \rangle^{-s}\|_\infty\,\|\varphi\| < \infty. \end{aligned}$$

We can now write

$$0 = [R_j(z)\,(H_j - z), \langle \mathbf{x} \rangle^{-s}]\,\varphi \;=\; R_j(z)\,[H_j, \langle \mathbf{x} \rangle^{-s}]\,\varphi + [R_j(z), \langle \mathbf{x} \rangle^{-s}]\,(H_j - z)\,\varphi,$$

which implies

$$[R_j(z), \langle \mathbf{x} \rangle^{-s}]\,(H_j - z)\,\varphi = -R_j(z)\,[H_j, \langle \mathbf{x} \rangle^{-s}]\,\varphi, \tag{3.16}$$

for all $\varphi \in \mathcal{D}(H_j)$. For any $\psi \in \mathcal{H}$ we can write $R_j(z)\,\psi$ instead of φ in (3.16), to obtain

$$[R_j(z), \langle \mathbf{x} \rangle^{-s}] = -R_j(z)\,[H_j, \langle \mathbf{x} \rangle^{-s}]\,R_j(z)\,, \tag{3.17}$$

as an equality of operators on $\mathcal{H}$. Now, we have

$$\begin{aligned} R_j(z)^2\,\langle \mathbf{x} \rangle^{-2s} &= R_j(z)\,\langle \mathbf{x} \rangle^{-2s}\,R_j(z) + R_j(z)\,[R_j(z), \langle \mathbf{x} \rangle^{-2s}] \\ &= R_j(z)\,\langle \mathbf{x} \rangle^{-2s}\,R_j(z) + R_j(z)^2\,2\,\langle \mathbf{x} \rangle^{-s}\,\mathrm{i}\,\boldsymbol{\sigma}\cdot\nabla\,\langle \mathbf{x} \rangle^{-s}\,R_j(z) \\ &= R_j(z)\,\langle \mathbf{x} \rangle^{-2s}\,R_j(z) + R_j(z)^2\,\langle \mathbf{x} \rangle^{-2s}\,\langle \mathbf{x} \rangle^{s}\,2\,\mathrm{i}\,\boldsymbol{\sigma}\cdot\nabla\,\langle \mathbf{x} \rangle^{-s}\,R_j(z), \end{aligned} \tag{3.18}$$

where we used (3.17) for $\langle \mathbf{x} \rangle^{-2s}$ at the second equality. From (3.18) we finally get

$$R_j(z)^2\,\langle \mathbf{x} \rangle^{-2s} = R_j(z)\,\langle \mathbf{x} \rangle^{-2s}\,R_j(z)\left(1 + 2\,s\,\frac{\mathrm{i}\,\boldsymbol{\sigma}\cdot\mathbf{x}}{\langle \mathbf{x} \rangle^2}\,R_j(z)\right)^{-1},$$

the invertibility of $\left(1 + 2\,s\,\frac{\mathrm{i}\,\boldsymbol{\sigma}\cdot\mathbf{x}}{\langle \mathbf{x} \rangle^2}\,R_j(z)\right)$ being consequence of $|\mathrm{Im}\,z| > 4\,s$. This means that $R_j(z)^2\,\langle \mathbf{x} \rangle^{-2s}$ differs from $R_j(z)\,\langle \mathbf{x} \rangle^{-2s}\,R_j(z)$ in a composition with a bounded operator and (3.13) follows. □

As a consequence of Lemmas 3.5 and 3.6 for the free operator we have

Corollary 3.7. *$\langle \mathbf{x} \rangle^{-s}\,R_0(\bar{z}\,)\,R_0(z)\,\langle \mathbf{x} \rangle^{-s}$ is a Hilbert-Schmidt operator for $s > \frac{1}{2}$ and $z \in \mathbb{C}$ with $|\mathrm{Im}\,z| > 4\,s$.*

Lemma 3.8. *Let $s \geqslant 0$ be such that $\boldsymbol{A} \in L^\infty_{-s}(\mathbb{R}^2, \mathbb{R}^2)$, $V \in L^\infty_{-s}(\mathbb{R}^2, \mathbb{R})$. Further let $k > \frac{1}{2}$ and $z \in \mathbb{C}$ with $|\mathrm{Im}\,z| > 4\,(s + k)$. Then $R(z)^2\,\langle \mathbf{x} \rangle^{-2(s+k)}$ is a Hilbert-Schmidt operator.*

Proof. By Lemma 3.6 it is enough to prove that $L := \langle \mathbf{x} \rangle^{-(s+k)}\,R(\bar{z}\,)\,R(z)\,\langle \mathbf{x} \rangle^{-(s+k)}$ is a Hilbert-Schmidt operator. By Lemma 3.3 we can write

$$\begin{aligned} L &= \big(R(z)\,\langle \mathbf{x} \rangle^{-(s+k)}\big)^*\,R(z)\,\langle \mathbf{x} \rangle^{-(s+k)} \\ &= (D^{-1})^*\,R(\bar{z}\,)\,(H_0 - H)\,\langle \mathbf{x} \rangle^{-(s+k)}\,R_0(\bar{z}\,)\,R_0(z)\,\langle \mathbf{x} \rangle^{-(s+k)}\,(H_0 - H)\,R(z)\,D^{-1} \\ &\quad + (D^{-1})^*\,R(\bar{z}\,)\,(H_0 - H)\,\langle \mathbf{x} \rangle^{-(s+k)}\,R_0(\bar{z}\,)\,R_0(z)\,\langle \mathbf{x} \rangle^{-(s+k)} \\ &\quad + \langle \mathbf{x} \rangle^{-(s+k)}\,R_0(\bar{z}\,)\,R_0(z)\,\langle \mathbf{x} \rangle^{-(s+k)}\,(H_0 - H)\,R(z)\,D^{-1} \\ &\quad + \langle \mathbf{x} \rangle^{-(s+k)}\,R_0(\bar{z}\,)\,R_0(z)\,\langle \mathbf{x} \rangle^{-(s+k)} \end{aligned}$$

3.4. Statement (3.14) is still true even if the kernels are not trivial. One can prove it using that the eigenvalues of $A\,A^*$ and of $A^*\,A$ are equal away from 0 [Tha92, Corollary 5.6] and that a compact operator is Hilbert-Schmidt if and only if the sum of the squares of its eigenvalues is finite.

as a sum of four operators, each of which is Hilbert-Schmidt for being a composition of bounded operators and the Hilbert-Schmidt operator $\langle \mathbf{x}\rangle^{-k} R_0(\bar{z}) R_0(z) \langle \mathbf{x}\rangle^{-k}$ (see Corollary 3.7). $\square$

Lemma 3.9. *Under the assumptions of Lemma 3.8, the operator $H_0 \langle \mathbf{x}\rangle^{-(3s+2k)} R(z)^3$ is Hilbert-Schmidt.*

Proof. We first remark that $\langle \mathbf{x}\rangle^{-\alpha} (R(z)\mathcal{H}) \subset \langle \mathbf{x}\rangle^{-\alpha} \mathcal{D}(H_0) \subset \mathcal{D}(H_0)$ for any $\alpha \geqslant 0$, so the operator $H_0 \langle \mathbf{x}\rangle^{-\alpha} R(z)$ is well defined on the whole $\mathcal{H}$.

Next notice that $H_0 R(z) \langle \mathbf{x}\rangle^{-s}$ is bounded by the weighted resolvent identity (Lemma 3.3): Left-composition with H_0 yields

$$H_0 R(z) \langle \mathbf{x}\rangle^{-s} = H_0 R_0(z) \langle \mathbf{x}\rangle^{-s} + H_0 R_0(z) \langle \mathbf{x}\rangle^{-s} (H_0 - H) R(z) D^{-1},$$

where D^{-1}, $\langle \mathbf{x}\rangle^{-s} (H_0 - H)$ and $H_0 R_0(z)$ are bounded operators, and hence $H_0 R(z) \langle \mathbf{x}\rangle^{-s}$ is bounded.

Let $L := H_0 \langle \mathbf{x}\rangle^{-(3s+2k)} R(z)^3$. We have

$$\begin{aligned} L &= H_0 R(z) \langle \mathbf{x}\rangle^{-(3s+2k)} R(z)^2 + H_0 \left[\langle \mathbf{x}\rangle^{-(3s+2k)}, R(z)\right] R(z)^2 \\ &= H_0 R(z) \langle \mathbf{x}\rangle^{-(3s+2k)} R(z)^2 - H_0 R(z) \left[\langle \mathbf{x}\rangle^{-(3s+2k)}, H\right] R(z)^3 \\ &= H_0 R(z) \langle \mathbf{x}\rangle^{-(3s+2k)} R(z)^2 - H_0 R(z)\, \mathrm{i}\, \boldsymbol{\sigma} \cdot \nabla \langle \mathbf{x}\rangle^{-(3s+2k)} R(z)^3 \\ &= H_0 R(z) \langle \mathbf{x}\rangle^{-s} \left(\langle \mathbf{x}\rangle^{-2(s+k)} R(z)^2 + (3s + 2k) \frac{\mathrm{i}\, \boldsymbol{\sigma} \cdot \mathbf{x}}{\langle \mathbf{x}\rangle^2} \langle \mathbf{x}\rangle^{-2(s+k)} R(z)^3 \right), \end{aligned} \tag{3.19}$$

where for the second identity we used the relation

$$\left[\langle \mathbf{x}\rangle^{-(3s+2k)}, R(z)\right] = -R(z) \left[\langle \mathbf{x}\rangle^{-(3s+2k)}, H\right] R(z)$$

proved in Lemma 3.6 as (3.17). The operator in parentheses in the last step of (3.19) is Hilbert-Schmidt because $\frac{\boldsymbol{\sigma} \cdot \mathbf{x}}{\langle \mathbf{x}\rangle^2}$ is bounded and $\langle \mathbf{x}\rangle^{-2(s+k)} R(z)^2 = \left(R(\bar{z})^2 \langle \mathbf{x}\rangle^{-2(s+k)}\right)^*$ is a Hilbert-Schmidt operator by Lemma 3.8, i.e. $H_0 \langle \mathbf{x}\rangle^{-(3s+2k)} R(z)$ is the composition of a Hilbert-Schmidt operator and the bounded $H_0 R(z) \langle \mathbf{x}\rangle^{-s}$. $\square$

Proof of Theorem 3.2. We now have all the ingredients we need to apply Theorem 2.2 and Theorem 2.4. The existence of a unitary equivalence in the form required in Theorem 2.2 was discussed in Note 2.3. We just need to find suitable Hilbert-Schmidt operators, which were already introduced in the previous lemmas.

Fix $k > \frac{1}{2}$ and $z \in \mathbb{C} \backslash \mathbb{R}$ with $|\operatorname{Im} z| > 4(s + k)$. For the choice

$$\gamma_1(h) := (h - z)^{-2} \quad \text{and} \quad T_1 := \langle \mathbf{x}\rangle^{2(s+k)}$$

Lemma 3.8 and Theorem 2.2 yield the existence of an expansion in generalized eigenfunctions[3.5]

$$u_1(\lambda) \in \mathcal{H}_-(T_1) = L^2_{-2(s+k)}.$$

With a different choice and Theorem 2.4 we gain information on the first weak derivatives. Let

$$\gamma_2(h) := (h - z)^{-3}, \; T_2 := \langle \mathbf{x}\rangle^{(3s+2k)}, \; S = H_0 - z\,.$$

We have that $\gamma_2(H) T_2^{-1} S$ is the restriction to $\mathcal{D}(S)$ of $\left((H_0 - \bar{z}) \langle \mathbf{x}\rangle^{-(3s+2k)} R(\bar{z})^3\right)^*$, which is Hilbert-Schmidt by Lemma 3.9. Hence, Theorem 2.4 provides an expansion in generalized eigenfunctions

$$u_2(\lambda) \in \mathcal{R}\left(\tilde{T}_2 (S^{-1})^*\right) = \langle \mathbf{x}\rangle^{(3s+2k)} R_0(\bar{z}) \mathcal{H} = H^1_{-(3s+2k)}. \qquad \square$$

3.5. If $T = \langle \mathbf{x}\rangle^{\alpha}$ for $\alpha \geqslant 0$, then the set $\mathcal{E} := \{\psi \in \mathcal{H}_+(T) \cap \mathcal{D}(H)$ with $H\psi \in \mathcal{H}_+(T)\}$ is a core for H and consequently the corresponding $u(\lambda)$ are generalized eigenfunctions of H. Indeed, any L^2 function with compact support is in $\mathcal{H}_+(T)$; this implies that $C_0^\infty \subset \mathcal{E}$ and, since C_0^∞ is a core for H (Lemma 3.1.b), so is $\mathcal{E}$.

3.3. Relationship between spectrum and generalized eigenvalues.

Once we have identified the generalized eigenvalues we would like to know how they are related to the spectrum. For a large class of Schrödinger operators the generalized eigenfunctions are polynomially bounded, and it holds that $\sigma(H)=\overline{\{\lambda|Hu=\lambda\,u \text{ has a polynomially bounded } \textit{solution}\}}$. We will adapt this result from [Sim82, §C.4 and §C.5] to our problem.

For convenience, in this section we shall call a generalized eigenfunction u of H corresponding to the generalized eigenvalue λ a **solution** of $Hu=\lambda u$. We say that a function u is $\boldsymbol{L^2}$**-polynomially bounded**, if $u\in L^2_{-s}$ for some $s\geqslant 0$.

Theorem 3.10. *Let H be the two-dimensional Dirac operator defined in §3.1, with $\boldsymbol{A}\in L^\infty_{-s}(\mathbb{R}^2,\mathbb{R}^2)$, $V\in L^\infty_{-s}(\mathbb{R}^2,\mathbb{R})$ for some $s\geqslant 0$. Then*

$$\sigma(H)=\overline{\{\lambda|Hu=\lambda\,u \textit{ has a } L^2\textit{-polynomially bounded solution}\}}.$$

Proof. We first prove the left to right inclusion[3.6]. Let E be the spectral family of H and U: $\mathcal{H}\to L^2(\mathbb{R}\times\mathbb{N},\rho)$ a unitary operator such that $UHU^*=h$, where $h(\lambda,j):=\lambda$ (see Note 2.3). Fix $\lambda_0\in\sigma(H)$. For $\varepsilon>0$ we have that the spectral projection $E(\lambda_0-\varepsilon,\lambda_0+\varepsilon)$ is different from zero. Further let $\Lambda_{(\lambda_0-\varepsilon,\lambda_0+\varepsilon)}:=\{(\lambda,j)\in\mathbb{R}\times\mathbb{N}:\lambda\in(\lambda_0-\varepsilon,\lambda_0+\varepsilon)\}$. Since $E(\lambda_0-\varepsilon,\lambda_0-\varepsilon)$ is unitarily equivalent to the multiplication by the characteristic function of $\Lambda_{(\lambda_0-\varepsilon,\lambda_0+\varepsilon)}$ in $L^2(\mathbb{R}\times\mathbb{N},\rho)$, it holds that $\rho(\Lambda_{(\lambda_0-\varepsilon,\lambda_0+\varepsilon)})>0$. On the other hand, by Theorem 3.2 we know that there exists a family $u(\lambda,j)$ of L^2-polynomially bounded functions which, in particular, satisfies b) in Theorem 2.2. That is, $u(\lambda,j)$ is a solution of $Hu(\lambda,j)=\lambda\,u(\lambda,j)$ for all $(\lambda,j)\notin N$, where N is some subset of $\mathbb{R}\times\mathbb{N}$ with $\rho(N)=0$. Because the set $\Lambda_{(\lambda_0-\varepsilon,\lambda_0+\varepsilon)}\backslash N$ has positive measure, we conclude that there exists $\lambda\in(\lambda_0-\varepsilon,\lambda_0+\varepsilon)$ such that $Hu=\lambda\,u$ has a L^2-polynomially bounded solution.

We now show the other inclusion. Assume $Hu=\lambda\,u$ has a solution $u\in L^2_{-\alpha}$, for $\alpha\geqslant 0$. We shall prove that λ is in $\sigma(H)$. Define the squares $Q_r:=\{\mathbf{x}\in\mathbb{R}^2:|x_i|\leqslant r \text{ for } i=1,2\}$, let

$$F(r):=\int_{Q_r}|u(\mathbf{x})|^2\,\mathrm{d}\mathbf{x}$$

and let $0\leqslant j_r\leqslant 1$ be a C_0^∞ function which is supported in Q_{r+1}, is equal to 1 on Q_r, and such that $\|\nabla j_r\|_\infty$ is uniformly bounded in r. Let $w_r:=j_r\,u/\|j_r\,u\|$. We will find normalized w_{r_n} such that $\|(H-\lambda)\,w_{r_n}\|\to 0$ as $n\to\infty$, which implies, by Weyl's criterion, that $\lambda\in\sigma(H)$.

Instead of polynomially bounded solutions like in the Schrödinger case we have L^2-polynomial boundedness, which is essentially the same in so far as it concerns this proof. We only need the following:

(*) *There exists r_0 such that for all $k\in\mathbb{N}$*

$$\int_{Q_{r_0+k}\backslash Q_{r_0+k-1}}|u(\mathbf{x})|^2\,\mathrm{d}\mathbf{x}\leqslant\int_{Q_{r_0+k}\backslash Q_{r_0+k-1}}\langle\mathbf{x}\rangle^\alpha\,\mathrm{d}\mathbf{x}.$$

We will prove (*) at the end. Using this property we conclude that there cannot exist $a>1$ such that $F(r_0+k)\geqslant a\,F(r_0+k-1)$ for all $k\in\mathbb{N}$, since we would then have $F(r_0+k)\geqslant a^k\,F(r_0)$ for all $k\in\mathbb{N}$, which contradicts (*):

The relation $F(r_0+k)\geqslant a^k\,F(r_0)$ together with (*) yields

$$\begin{aligned} a^k\int_{Q_{r_0}}|u|^2 &\leqslant \int_{Q_{r_0+k}}|u|^2\\ &= \int_{Q_{r_0}}|u|^2+\int_{Q_{r_0+k}\backslash Q_{r_0}}|u|^2\\ &\leqslant \int_{Q_{r_0}}|u|^2+\int_{Q_{r_0+k}\backslash Q_{r_0}}\langle\mathbf{x}\rangle^\alpha, \end{aligned}$$

and hence

$$(a^k-1)\int_{Q_{r_0}}|u|^2\leqslant\int_{Q_{r_0+k}\backslash Q_{r_0}}\langle\mathbf{x}\rangle^\alpha,$$

3.6. That the spectrum of a self-adjoint operator is contained in the closure of the set of its generalized eigenvalues holds whenever Theorem 2.2 is applicable.

the left hand side growing like a^k and the right hand side like $k^{\alpha+2}$ as k grows to infinity, which means that the inequality cannot hold for arbitrarily big values of k.

Then, for any $a>1$ there exists $k\in\mathbb{N}$ such that $F(r_0+k)<a\,F(r_0+k-1)$ and picking $a_n=1+1/n$ for each $n\in\mathbb{N}$, we find an non-decreasing sequence k_n with $F(r_0+k_n)<a_n\,F(r_0+k_n-1)$. For the sequence of radii $r_n:=r_0+k_n-1$ we have

$$\frac{F(r_n+1)}{F(r_n)}\to 1 \tag{3.20}$$

as $n\to\infty$. Now

$$(H-\lambda)\,j_r\,u=j_r\,(H-\lambda)\,u+[H,j_r]\,u=-\mathrm{i}\,(\boldsymbol{\sigma}\cdot\nabla j_r)\,u,$$

and since the ∇j_r are uniformly bounded and supported in $Q_{r+1}\backslash Q_r$, we obtain

$$\|(H-\lambda)\,j_r\,u\|^2=\|(\boldsymbol{\sigma}\cdot\nabla j_r)\,u\|\leqslant C\int_{Q_{r+1}\backslash Q_r}|u|^2,$$

for all r. From this and $F(r_n)\leqslant\|j_r\,u\|^2$ follows, for each r_n, that

$$\begin{aligned}\|(H-\lambda)\,w_{r_n}\|^2 &\leqslant C\,[F(r_n+1)-F(r_n)]/F(r_n)\\ &= C\left[\frac{F(r_n+1)}{F(r_n)}-1\right],\end{aligned}$$

which converges to 0 by (3.20).

We finish with the proof of (*). Assume it is false. Then for all $\rho>0$ there exists $k(\rho)\in\mathbb{N}$ such that

$$\int_{Q_{\rho+k(\rho)}\backslash Q_{\rho+k(\rho)-1}}|u|^2>\int_{Q_{\rho+k(\rho)}\backslash Q_{\rho+k(\rho)-1}}\langle\mathbf{x}\rangle^\alpha.$$

A direct computation shows that

$$\int_{Q_\rho\backslash Q_{\rho-1}}\langle\mathbf{x}\rangle^\alpha\,\mathrm{d}\mathbf{x}\geqslant\sup_{\mathbf{x}\in Q_\rho\backslash Q_{\rho-1}}\langle\mathbf{x}\rangle^\alpha \tag{3.21}$$

for all ρ large enough. Let ρ_0 be one such ρ, large enough for (3.21) to hold, and let $\rho_{n+1}:=\rho_n+k(\rho_n)$. Then we have, for all $n\geqslant 1$,

$$\int_{Q_{\rho_n}\backslash Q_{\rho_n-1}}|u|^2>\int_{Q_{\rho_n}\backslash Q_{\rho_n-1}}\langle\mathbf{x}\rangle^\alpha$$

and by (3.21) this implies

$$\int_{Q_{\rho_n}\backslash Q_{\rho_n-1}}\frac{|u|^2}{\langle\mathbf{x}\rangle^\alpha}\geqslant\frac{\int_{Q_{\rho_n}\backslash Q_{\rho_n-1}}|u|^2}{\sup_{\mathbf{x}\in Q_{\rho_n}\backslash Q_{\rho_n-1}}\langle\mathbf{x}\rangle^\alpha}\geqslant\frac{\int_{Q_{\rho_n}\backslash Q_{\rho_n-1}}|u|^2}{\int_{Q_{\rho_n}\backslash Q_{\rho_n-1}}\langle\mathbf{x}\rangle^\alpha}>1.$$

Because the sets $Q_{\rho_n}\backslash Q_{\rho_n-1}$ are pairwise disjoint by the choice of ρ_n, we conclude

$$\begin{aligned}\int_{\mathbb{R}^2}\frac{|u|^2}{\langle\mathbf{x}\rangle^\alpha} &\geqslant \sum_{n=1}^\infty\int_{Q_{\rho_n}\backslash Q_{\rho_n-1}}\frac{|u|^2}{\langle\mathbf{x}\rangle^\alpha}\\ &> \sum_{n=1}^\infty 1=\infty,\end{aligned}$$

which contradicts the integrability of $|u|^2\,\langle\mathbf{x}\rangle^{-\alpha}$. □

3.4. Comments.

A possible application of such expansions is the following. Assume we could prove for some particular Dirac operator H that every solution $u\in L^2_{-\alpha}$ of the equation $H u=\lambda\ u$ is actually in L^2, for instance by proving exponential decay of such a solution. Then the generalized eigenfunction u is in fact an eigenfunction, and the relationship $\sigma(H)=\overline{\{\lambda|Hu=\lambda\,u\text{ has a }L^2\text{-polynomially bounded solution}\}}$ (Theorem 3.10) implies that the spectrum of H is pure point. This kind of argument has often been used for Schrödinger operators in the proofs of Anderson localization; see, for example, [FMSS85], [DK89].

4. 1-D massless Dirac operator: dynamical estimates through an expansion in generalized eigenfunctions

The aim of this section is to give an explicit expansion in generalized eigenfunctions of the one-dimensional massless Dirac operator with external potential V and use this expansion to study its dynamical behaviour. This can be achieved just by studying the free operator, since the massless Dirac operator with potential is unitarily equivalent to the the massless free one (see §4.1 below). However we use instead Weidmann's method for ordinary differential operators (§2.2) for one main reason: as a preparation for the case with positive mass. We believe this method could help in this more complicated setting, which we intend to study in a near future. We find therefore convenient and also interesting to see how this method works in this particular, easier example.

The expansion in generalized eigenfunctions of the 1-dimensional massless Dirac operator using Weidmann's method is given in §4.2. We later use this expansion in §4.4 to study the dynamics: we compute $x_\psi^2(t) := \langle \mathrm{e}^{-\mathrm{i}Ht}\,\psi(x), x^2\,\mathrm{e}^{-\mathrm{i}Ht}\,\psi(x)\rangle$ –which represents the (expected value of the) square of the position of ψ at the time t– and obtain ballistic motion[4.1] of the massless Dirac particles independently of the external potential V. Note that $x_\psi^2(t)$ does not make sense for any ψ, but only if $\mathrm{e}^{-\mathrm{i}Ht}\,\psi(x) \in \mathcal{D}(x^2)$. We deal with this domain issue in §4.3.

4.1. Definition of the 1-D operator.

The 1-dimensional massless free Dirac operator H_0 is defined as the self-adjoint closure in $L^2(\mathbb{R}, \mathbb{C}^2)$ of the essentially self-adjoint operator[4.2]

$$\tilde{H}_0 := -\mathrm{i}\,c\,\sigma_1\,\frac{\mathrm{d}}{\mathrm{d}x}$$

on $C_0^\infty(\mathbb{R}, \mathbb{C}^2)$, where

$$\sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

With an electric potential $V \in L^1_{\mathrm{loc}}(\mathbb{R})$, $\tilde{H} := \tilde{H}_0 + V$ on $C_0^\infty(\mathbb{R}, \mathbb{C}^2)$ is also essentially self-adjoint and we define H as its closure in $L^2(\mathbb{R}, \mathbb{C}^2)$. Actually, see [Sch10, Proposition 1.1], $\tilde{H}$ is unitarily equivalent to $\tilde{H}_0$:

$$\mathrm{e}^{-\mathrm{i}\frac{1}{c}\sigma_1 q(x)}\left(-\mathrm{i}\,c\,\sigma_1\,\frac{\mathrm{d}}{\mathrm{d}x}\right)\mathrm{e}^{\mathrm{i}\frac{1}{c}\sigma_1 q(x)} = -\mathrm{i}\,c\,\sigma_1\,\frac{\mathrm{d}}{\mathrm{d}x} + V(x), \tag{4.1}$$

where $q(x) := \int_0^x V(\xi)\,\mathrm{d}\,\xi$ is locally absolutely continuous. Therefore it inherits the spectral properties of $\tilde{H}_0$, in particular it is essentially self-adjoint.

Throughout Section 4 $\mathcal{H}$ denotes the Hilbert space $L^2(\mathbb{R}, \mathbb{C}^2)$, $V \in L^1_{\mathrm{loc}}(\mathbb{R}, \mathbb{R})$ the electric potential, and H_0 resp. H the self-adjoint extensions in $\mathcal{H}$ of $\tilde{H}_0$ resp. $\tilde{H}$.

4.2. Expansion in generalized eigenfunctions by Weidmann's method.

Theorem 4.1. *Let H be the 1-dimensional massless Dirac operator defined in 4.1. Let*

$$(F\psi)(\lambda) = \underset{N\to\infty}{l.i.m.}\,\frac{1}{\sqrt{2\,\pi\,c}}\int_{-N}^{N}\mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1(\lambda x - q(x))}\,\psi(x)\,\mathrm{d}\,x,$$

where $q(x) := \int_0^x V(\xi)\,\mathrm{d}\,\xi$. Then $F\colon \mathcal{H} \to \mathcal{H}$ is a spectral representation of H with inverse

$$(F^{-1}\,\phi)(x) = \underset{N\to\infty}{l.i.m.}\,\frac{1}{\sqrt{2\,\pi\,c}}\int_{-N}^{N}\mathrm{e}^{\frac{\mathrm{i}}{c}\sigma_1(\lambda x - q(x))}\,\phi(\lambda)\,\mathrm{d}\,\lambda.$$

4.1. By **ballistic motion** we mean that $x_\psi^2(t) \leqslant C_\psi\,t^2$ for some constant C_ψ depending only on ψ. Our result is, however, an identity and not only an upper bound.

4.2. The same argument as for the 2-dimensional case (see Lemma 3.1.a) proves that $\tilde{H}_0$ is essentially self-adjoint.

This can be proved directly by finding a spectral representation of the free operator via the Fourier transform and then using the relation (4.1), but we will prove it instead by the method given in §2.2, which provides explicit formulae for computing a spectral representation of ordinary differential operators when the resolvent kernel is known.

The solutions of $(H-z)\,u=0$ have the form $\mathrm{e}^{\frac{\mathrm{i}}{c}\sigma_1(zx-q(x))}\,u_0$. Since this is a system of two ordinary differential equations of order one, there exist for each $z\in\mathbb{C}$ two linearly independent solutions. We choose

$$u_1(x,z):=\frac{1}{\sqrt{4\,\pi\,c}}\,\mathrm{e}^{\frac{\mathrm{i}}{c}\sigma_1(zx-q(x))}\begin{pmatrix}1\\1\end{pmatrix},\quad u_2(x,z):=\frac{1}{\sqrt{4\,\pi\,c}}\,\mathrm{e}^{\frac{\mathrm{i}}{c}\sigma_1(zx-q(x))}\begin{pmatrix}1\\-1\end{pmatrix}.$$

Note that $u_i(x,z)$ are entire functions of z, for $i=1,2$. Therefore we can use Theorem 2.5 to find the following spectral representation in terms of the u_i:

Lemma 4.2. *The unitary operator* $U=(U_1,U_2)\colon\mathcal{H}\to L^2(\mathbb{R},\mathbb{C})\oplus L^2(\mathbb{R},\mathbb{C})$ *given by*

$$(U_i\,\psi)(\lambda)=\underset{N\to\infty}{\mathrm{l.i.m.}}\int_{-N}^{N}(u_i(x,\lambda),\psi(x))\,\mathrm{d}x,\quad i=1,2$$

is a spectral representation of H *with inverse*

$$(U^{-1}\,\phi)(x)=\underset{N\to\infty}{\mathrm{l.i.m.}}\int_{-N}^{N}u_1(x,\lambda)\,\phi_1(\lambda)+u_2(x,\lambda)\,\phi_2(\lambda)\,\mathrm{d}\lambda.$$

Proof. Let

$$P_1=\frac{1}{2}\begin{pmatrix}1&1\\1&1\end{pmatrix},\quad P_2=\frac{1}{2}\begin{pmatrix}1&-1\\-1&1\end{pmatrix}$$

be the orthogonal projections in $\mathbb{C}^2$ onto the eigenspaces of σ_1, generated by $(1,1)$ and $(1,-1)$, respectively. For $z\in\mathbb{C}\backslash\mathbb{R}$, if $\operatorname{Im}z>0$ we have

$$\begin{aligned}(H-z)^{-1}\,\psi(x)&=\frac{\mathrm{i}}{c}\sigma_1\int_{-\infty}^{x}\mathrm{e}^{\frac{\mathrm{i}}{c}\sigma_1(zx-q(x))}\,\mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1(zy-q(y))}\,P_1\,\psi(y)\,\mathrm{d}y\\&\quad-\frac{\mathrm{i}}{c}\sigma_1\int_{x}^{\infty}\mathrm{e}^{\frac{\mathrm{i}}{c}\sigma_1(zx-q(x))}\,\mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1(zy-q(y))}\,P_2\,\psi(y)\,\mathrm{d}y,\end{aligned}\tag{4.2}$$

and if $\operatorname{Im}z<0$

$$\begin{aligned}(H-z)^{-1}\,\psi(x)&=-\frac{\mathrm{i}}{c}\sigma_1\int_{x}^{\infty}\mathrm{e}^{\frac{\mathrm{i}}{c}\sigma_1(zx-q(x))}\,\mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1(zy-q(y))}\,P_1\,\psi(y)\,\mathrm{d}y\\&\quad+\frac{\mathrm{i}}{c}\sigma_1\int_{-\infty}^{x}\mathrm{e}^{\frac{\mathrm{i}}{c}\sigma_1(zx-q(x))}\,\mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1(zy-q(y))}\,P_2\,\psi(y)\,\mathrm{d}y.\end{aligned}\tag{4.3}$$

We comment on how to prove this fact at the end $(*)$. Using now that $\sigma_1\,P_1=P_1\,\sigma_1=P_1$ and $\sigma_1\,P_2=P_2\,\sigma_1=-P_2$ we arrive at

$$\begin{aligned}\sigma_1\,\mathrm{e}^{\frac{\mathrm{i}}{c}\sigma_1(zx-q(x))}\,\mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1(zy-q(y))}\,P_1&=\mathrm{e}^{\frac{\mathrm{i}}{c}\sigma_1(zx-q(x))}\,P_1\,\mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1(zy-q(y))}\\&=2\,\pi\,c\,u_1(x,z)\,\overline{u_1(y,\bar{z})}\end{aligned}$$

and

$$\begin{aligned}\sigma_1\,\mathrm{e}^{\frac{\mathrm{i}}{c}\sigma_1(zx-q(x))}\,\mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1(zy-q(y))}\,P_2&=-\mathrm{e}^{\frac{\mathrm{i}}{c}\sigma_1(zx-q(x))}\,P_2\,\mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1(zy-q(y))}\\&=-2\,\pi\,c\,u_2(x,z)\,\overline{u_2(y,\bar{z})},\end{aligned}$$

that is, the resolvent kernel is, if $\operatorname{Im}z>0$,

$$R(x,y,z)=\begin{cases}2\,\pi\,\mathrm{i}\,u_1(x,z)\,\overline{u_1(y,\bar{z})}&\text{for }y\leqslant x\\2\,\pi\,\mathrm{i}\,u_2(x,z)\,\overline{u_2(y,\bar{z})}&\text{for }y>x\end{cases},$$

and if $\operatorname{Im}z<0$

$$R(x,y,z)=\begin{cases}-2\,\pi\,\mathrm{i}\,u_2(x,z)\,\overline{u_2(y,\bar{z})}&\text{for }y\leqslant x\\-2\,\pi\,\mathrm{i}\,u_1(x,z)\,\overline{u_1(y,\bar{z})}&\text{for }y>x\end{cases}.$$

In the notation of §2.2 this implies that, for $\operatorname{Im} z > 0$, $m_{11}^{+}(z) = m_{22}^{-}(z) = 2\,\pi\,\mathrm{i}$, and $m_{ij}^{\pm}(z) = 0$ otherwise. With (2.1) we obtain $\rho(\lambda) = \lambda\,\mathbb{I}$. Finally by Theorem 2.5 we arrive at the desired spectral representation.

(∗) We now prove that the resolvent is in fact given by (4.2) resp. (4.3) for $\operatorname{Im} z > 0$ resp. $\operatorname{Im} z < 0$. First notice that the distinction for $\operatorname{Im} z > 0$ and $\operatorname{Im} z < 0$ is necessary for the integrals to converge:

Because $\sigma_1\,P_1\,\psi = P_1\,\psi$ and $\sigma_1\,P_2\,\psi = -P_2\,\psi$, we have

$$\mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1 z y}\,P_1\,\psi(y) = \mathrm{e}^{-\frac{\mathrm{i}}{c} z y}\,P_1\,\psi(y) \quad \text{and} \quad \mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1 z y}\,P_2\,\psi(y) = \mathrm{e}^{\frac{\mathrm{i}}{c} z y}\,P_2\,\psi(y).$$

Therefore, the function $\mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1 z y}\,P_1\,\psi(y)$ in $(-\infty, x)$ is in general not integrable if $\operatorname{Im} z < 0$, but it is integrable if $\operatorname{Im} z > 0$. One should treat the 3 other cases similarly.

We now check that the resolvent is given by (4.2) for $\operatorname{Im} z > 0$; the other case is analogous. For simplicity, let us introduce the operators

$$(A_1\,\psi)(x) := \frac{\mathrm{i}}{c}\,\sigma_1 \int_{-\infty}^{x} \mathrm{e}^{\frac{\mathrm{i}}{c}\sigma_1(zx - q(x))}\,\mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1(zy - q(y))}\,P_1\,\psi(y)\,\mathrm{d}y,$$

$$(A_2\,\psi)(x) := -\frac{\mathrm{i}}{c}\,\sigma_1 \int_{x}^{\infty} \mathrm{e}^{\frac{\mathrm{i}}{c}\sigma_1(zx - q(x))}\,\mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1(zy - q(y))}\,P_2\,\psi(y)\,\mathrm{d}y.$$

We won't specify their domain now, but the calculations below show in particular that $A_i\colon \mathcal{H} \to \mathcal{D}(H)$. What we claim in (4.2) is thus that $(H - z)^{-1}\,\psi = A_1\,\psi + A_2\,\psi$. We first prove $(H - z)\,(A_1 + A_2)\,\psi = \psi$:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}x}\,(A_1\,\psi)(x) &= \frac{\mathrm{i}}{c}\,\sigma_1\,\frac{\mathrm{d}}{\mathrm{d}x}\left(\mathrm{e}^{\frac{\mathrm{i}}{c}\sigma_1(zx - q(x))} \int_{-\infty}^{x} \mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1(zy - q(y))}\,P_1\,\psi(y)\,\mathrm{d}y\right)\\
&= \frac{\mathrm{i}}{c}\,\sigma_1\,(z - V(x))\,(A_1\,\psi)(x) + \frac{\mathrm{i}}{c}\,\sigma_1\,\mathrm{e}^{\frac{\mathrm{i}}{c}\sigma_1(zx - q(x))}\,\mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1(zx - q(x))}\,P_1\,\psi(x)\\
&= \frac{\mathrm{i}}{c}\,\sigma_1\,[(z - V(x))\,(A_1\,\psi)(x) + P_1\,\psi(x)].
\end{aligned}$$

Hence, $(H_0 + V(x) - z)\,(A_1\,\psi)(x) = P_1\,\psi(x)$. For $A_2\,\psi$ it is proved analogously that $(H_0 + V(x) - z)\,(A_2\,\psi)(x) = P_2\,\psi(x)$. Adding up both identities we conclude that

$$(H - z)\,(A_1\,\psi + A_2\,\psi) = P_1\,\psi + P_2\,\psi = \psi.$$

It remains to prove that $(A_1 + A_2)\,(H - z)\,\psi = \psi$, for $\psi \in \mathcal{D}(H)$. Integrating by parts we get

$$\begin{aligned}
(A_1\,\psi')(x) &= \frac{\mathrm{i}}{c}\,\sigma_1\,\mathrm{e}^{\frac{\mathrm{i}}{c}\sigma_1(zx - q(x))}\Big(\mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1(zx - q(x))}\,P_1\,\psi(x)\\
&\quad + \int_{-\infty}^{x} \frac{\mathrm{i}}{c}\,\sigma_1\,(z - V(y))\,\mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1(zy - q(y))}\,P_1\,\psi(y)\,\mathrm{d}y\Big)\\
&= \frac{\mathrm{i}}{c}\,\sigma_1\,P_1\,\psi(x) + \frac{\mathrm{i}}{c}\,\sigma_1\,(A_1\,(z - V)\,\psi)(x),
\end{aligned}$$

which implies that

$$A_1\,(H - z)\,\psi = -\mathrm{i}\,c\,\sigma_1\,A_1\,\psi' + A_1\,(V - z)\,\psi = P_1\,\psi.$$

Similarly, $A_2\,(H - z)\,\psi = P_2\,\psi$ and hence $(A_1 + A_2)\,(H - z)\,\psi = \psi$. From this follows that the resolvent is given by (4.2) for $\operatorname{Im} z > 0$. □

Now we finish the proof of Theorem 4.1. Notice that

$$(U\psi)(\lambda) = \operatorname*{l.i.m.}_{N\to\infty} \frac{1}{\sqrt{2\,\pi\,c}} \int_{-N}^{N} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1(\lambda x - q(x))}\,\psi(x)\,\mathrm{d}x$$

and

$$(U^{-1}\,\phi)(x) = \operatorname*{l.i.m.}_{N\to\infty} \frac{1}{\sqrt{2\,\pi\,c}} \int_{-N}^{N} \mathrm{e}^{\frac{\mathrm{i}}{c}\sigma_1(\lambda x - q(x))}\,\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \phi(\lambda)\,\mathrm{d}\lambda.$$

Hence $F = B\,U$, $F^{-1} = U^{-1}\,B^{-1}$, where $B = B^{-1} = \frac{1}{\sqrt{2}}\left(\begin{smallmatrix} 1 & 1 \\ 1 & -1 \end{smallmatrix}\right)$ is just a unitary change of basis in $\mathbb{C}^2$, and therefore F is also a spectral representation of H.

4.3. Invariance of $\mathcal{D}(x^2)$ under the time evolution.

The next theorem shows that the time evolution operator leaves the domain of the multiplication by x^n invariant and yields also an upper bound for $x_\psi^{2n}(t) = \langle \mathrm{e}^{-\mathrm{i}Ht}\,\psi(x), x^{2n}\,\mathrm{e}^{-\mathrm{i}Ht}\,\psi(x)\rangle$. We just prove the result for the 1-dimensional massless case, but it holds for higher dimensions (2 and 3) and their massive versions too. The proof for these other cases is almost identical; see [Tha92, Theorem 8.5].

Theorem 4.3. *Let H be the 1-dimensional massless Dirac operator defined in §4.1. Then*

$$\mathrm{e}^{-\mathrm{i}Ht}\,\mathcal{D}(x^n) \subset \mathcal{D}(x^n), \quad \text{for } n = 0, 1, 2, \ldots$$

and there are constants $k_n(\psi)$ depending only on n and ψ such that

$$\|x^n\,\mathrm{e}^{-\mathrm{i}Ht}\,\psi\| \leqslant k_n(\psi)\,(1 + c\,|t|)^n, \quad \text{for all } \psi \in \mathcal{D}(x^n).$$

For $n = 1$, this upper bound implies that the particle cannot escape faster than the velocity of light. The conclusion of this theorem is thus false in non-relativistic quantum mechanics.

Proof. We proceed inductively. For $n = 0$ the time evolution leaves $\mathcal{D}(x^0) = \mathcal{H}$ clearly invariant and the bound holds with $k_0(\psi) = \|\psi\|$. Assume it is true for $n - 1$ and define for $\varepsilon > 0$ the regularization[4.3]

$$B_\varepsilon(x) := \frac{x^n}{(1 + \varepsilon\,x^{2n})^{1/2}}, \quad x \in \mathbb{R}.$$

Let B_ε denote the multiplication operator by $B_\varepsilon(x)$. For each $\varepsilon > 0$ this operator is bounded and, since $B_\varepsilon'(x)$ is also bounded, $B_\varepsilon\,\psi \in \mathcal{D}(H)$ whenever $\psi \in \mathcal{D}(H)$.

Let $\varphi \in C_0^\infty(\mathbb{R}^2, \mathbb{C}^2) \subset \mathcal{D}(H) \cap \mathcal{D}(x^n)$. It holds, by Stone's Theorem [RS80, Theorem VIII.17], that

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{\mathrm{i}Ht}\,B_\varepsilon\,\mathrm{e}^{-\mathrm{i}Ht}\,\varphi = \mathrm{i}\,\mathrm{e}^{\mathrm{i}Ht}\,[H, B_\varepsilon]\,\mathrm{e}^{-\mathrm{i}Ht}\,\varphi.$$

Integrating from 0 to t we get

$$\mathrm{e}^{\mathrm{i}Ht}\,B_\varepsilon\,\mathrm{e}^{-\mathrm{i}Ht}\,\varphi = B_\varepsilon\,\varphi + \mathrm{i}\int_0^t \mathrm{e}^{\mathrm{i}Hs}\,[H, B_\varepsilon]\,\mathrm{e}^{-\mathrm{i}Hs}\,\varphi\,\mathrm{d}s. \tag{4.4}$$

We can actually extend this identity on $C_0^\infty(\mathbb{R}^2, \mathbb{C}^2)$ by continuity to all $\psi \in \mathcal{H}$, since $[H, B_\varepsilon] = -\mathrm{i}\,c\,\sigma_1\,B_\varepsilon'(x)$ is bounded and therefore

$$\left\|\int_0^t \mathrm{e}^{\mathrm{i}Hs}\,[H, B_\varepsilon]\,\mathrm{e}^{-\mathrm{i}Hs}\,\varphi_n\,\mathrm{d}s - \int_0^t \mathrm{e}^{\mathrm{i}Hs}\,[H, B_\varepsilon]\,\mathrm{e}^{-\mathrm{i}Hs}\,\psi\,\mathrm{d}s\right\| \leqslant |t|\,\|[H, B_\varepsilon]\|\,\|\varphi_n - \psi\|\,\mathrm{d}s \to 0$$

if $\varphi_n \to \psi$ in $\mathcal{H}$. Then, taking norms in (4.4) for $\psi \in \mathcal{D}(x^n)$ and using the induction hypothesis, we have

$$\begin{aligned}
\|B_\varepsilon\,\mathrm{e}^{-\mathrm{i}Ht}\,\psi\| &\leqslant \|B_\varepsilon\,\psi\| + \int_0^t \left\|c\,\sigma_1 \frac{n\,x^{n-1}}{(1 + \varepsilon\,x^{2n})^{3/2}}\,\mathrm{e}^{-\mathrm{i}Hs}\,\psi\right\|\mathrm{d}s \\
&\leqslant \|x^n\,\psi\| + \int_0^t c\,n\,\|x^{n-1}\,\mathrm{e}^{-\mathrm{i}Hs}\,\psi\|\,\mathrm{d}s \\
&\leqslant \|x^n\,\psi\| + \int_0^t c\,n\,k_{n-1}(\psi)(1 + c\,|t|)^{n-1}\,\mathrm{d}s \\
&\leqslant k_n(\psi)\,(1 + c\,|t|)^n,
\end{aligned}$$

4.3. We changed the definition of $B_\varepsilon(x)$ from Thaller's proof so it does not have singularities when $d = 1$ and n is odd.

so letting $\varepsilon \to 0$ in the left-hand side, $\|x^n\, \mathrm{e}^{-\mathrm{i}Ht}\, \psi\| \leqslant k_n(\psi)\ (1 + c\ |t|)^n$ and consequently $\mathrm{e}^{-\mathrm{i}Ht}\, \psi \in \mathcal{D}(x^n)$. □

4.4. Dynamics.

We are ready to study the dynamics of the 1-dimensional massless Dirac operator using the spectral representation F given in Theorem 4.1. We compute the expected value of the square of the position of $\psi \in \mathcal{D}(x^2)$ at the time t, that is, we compute $x_\psi^2(t) := \langle \mathrm{e}^{-\mathrm{i}Ht}\, \psi(x), x^2\, \mathrm{e}^{-\mathrm{i}Ht}\, \psi(x)\rangle$. From the bound in Theorem 4.3 we already know the motion is ballistic. Here we find not only a bound but an identity, independent of the external potential V[4.4].

We also introduce the notation $\psi(x,t) := \mathrm{e}^{-\mathrm{i}Ht}\, \psi(x)$.

Theorem 4.4. *For $\psi \in \mathcal{D}(x^2)$ it holds*

$$\begin{aligned}\langle \psi(x,t), x^2\, \psi(x,t)\rangle &= c^2\, t^2\, \|\psi\|^2 + 2\, c\, t\, (\langle P_1\, \psi(x), x\, P_1\, \psi(x)\rangle - \langle P_2\, \psi(x), x\, P_2\, \psi(x)\rangle) \\ &\quad + \langle \psi(x), x^2\, \psi(x)\rangle,\end{aligned} \tag{4.5}$$

where $P_1 = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$, $P_2 = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$ are the orthogonal projections onto the eigenspaces of σ_1 with eigenvalues 1 and -1, respectively.

Proof. First notice that $\mathcal{D}(x^2) \subset \mathcal{D}(x)$, and also by Theorem 4.3 $\psi(x,t) \in \mathcal{D}(x^2)$, so every term in (4.5) makes sense. Moreover, by the dominated convergence theorem,

$$\begin{aligned}\langle \psi(x,t), x^2\, \psi(x,t)\rangle &= \lim_{\varepsilon \to 0_+} \left\langle \psi(x,t), x^2\, \mathrm{e}^{-\varepsilon x^2}\, \psi(x,t)\right\rangle \\ &= \lim_{\varepsilon \to 0_+} -\frac{\mathrm{d}}{\mathrm{d}\varepsilon} \left\langle \psi(x,t), \mathrm{e}^{-\varepsilon x^2}\, \psi(x,t)\right\rangle \\ &=: \lim_{\varepsilon \to 0_+} -\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\, f_\psi(\varepsilon, t).\end{aligned}$$

We will now use the spectral representation F defined in Theorem 4.1 to compute $f_\psi(\varepsilon, t)$ as follows:

$$\begin{aligned}f_\psi(\varepsilon,t) &= \left\langle F^{-1}\, F\psi(x,t), \mathrm{e}^{-\varepsilon x^2}\, F^{-1}\, F\psi(x,t)\right\rangle \\ &= \lim_{N,M \to \infty} \left\langle F^{-1}\, \chi_{[-N,N]}\, \mathrm{e}^{-\mathrm{i}\lambda t}\, F\psi, \mathrm{e}^{-\varepsilon x^2}\, F^{-1}\, \chi_{[-M,M]}\, \mathrm{e}^{-\mathrm{i}\mu t}\, F\psi\right\rangle,\end{aligned}$$

by the continuity of the escalar product. Since the integrands are in L^1 with respect to each variable x, λ and μ we may exchange the order of integration and obtain

$$f_\psi(\varepsilon,t) = \frac{1}{2\pi c} \lim_{N,M \to \infty} \int_{-N}^{N}\int_{-M}^{M}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}(\lambda-\mu)t}\, \overline{F\psi(\lambda)}\, \mathrm{e}^{-\frac{\mathrm{i}}{c}\sigma_1(\lambda-\mu)x}\, F\psi(\mu)\, \mathrm{e}^{-\varepsilon x^2}\, \mathrm{d}x\, \mathrm{d}\mu\, \mathrm{d}\lambda.$$

We can write the Hilbert space as the orthogonal sum $\mathcal{H} = P_1\mathcal{H} \oplus P_2\mathcal{H}$. Let us first assume $\psi \in P_1\mathcal{H}$. Then we have $F\psi \in P_1\mathcal{H}$ as well and we compute

$$\begin{aligned}f_\psi(\varepsilon,t) &= \frac{1}{2\pi c} \lim_{N,M \to \infty} \int_{-N}^{N}\int_{-M}^{M}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}(\lambda-\mu)t}\, \overline{F\psi(\lambda)}\, F\psi(\mu)\, \mathrm{e}^{-\varepsilon x^2}\, \mathrm{e}^{-\frac{\mathrm{i}}{c}(\lambda-\mu)x}\, \mathrm{d}x\, \mathrm{d}\mu\, \mathrm{d}\lambda \\ &= \frac{1}{\sqrt{2\pi}\, c} \lim_{N,M \to \infty} \int_{-N}^{N}\int_{-M}^{M} \mathrm{e}^{\mathrm{i}(\lambda-\mu)t}\, \overline{F\psi(\lambda)}\, F\psi(\mu)\, \left(\mathcal{F}\mathrm{e}^{-\varepsilon x^2}\right)\left(\frac{\lambda-\mu}{c}\right) \mathrm{d}\mu\, \mathrm{d}\lambda \\ &= \frac{1}{\sqrt{2\pi}\, c}\, \frac{1}{\sqrt{2\,\varepsilon}} \lim_{N,M \to \infty} \int_{-N}^{N}\int_{-M}^{M} \mathrm{e}^{\mathrm{i}(\lambda-\mu)t}\, \overline{F\psi(\lambda)}\, F\psi(\mu)\, \mathrm{e}^{-\left(\frac{\lambda-\mu}{c}\right)^2 \frac{1}{4\varepsilon}}\, \mathrm{d}\mu\, \mathrm{d}\lambda,\end{aligned}$$

where $\mathcal{F}$ in the second equality denotes the Fourier transform. If $\psi \in P_2\mathcal{H}$ –and as a consequence so is $F\psi$– we obtain $\mathrm{e}^{\frac{\mathrm{i}}{c}(\lambda-\mu)x}$ and $\left(\mathcal{F}\mathrm{e}^{-\varepsilon x^2}\right)\left(\frac{-(\lambda-\mu)}{c}\right)$ in the first and second identities instead, but this leads to the same conclusion since $\left(\mathcal{F}\mathrm{e}^{-\varepsilon x^2}\right)(k) = \left(\mathcal{F}\mathrm{e}^{-\varepsilon x^2}\right)(-k)$.

4.4. Note that one can conclude a priori that the result will not depend on the external potential: We have $H = A^*\, H_0\, A$, where A is the unitary operator $\exp\left(\mathrm{i}\, \frac{1}{c}\, \sigma_1\, q(x)\right)$; see (4.1). Therefore, $\mathrm{e}^{-\mathrm{i}Ht} = A^*\, \mathrm{e}^{-\mathrm{i}H_0 t}\, A = \mathrm{e}^{-\mathrm{i}H_0 t}$, the last step because A and $\mathrm{e}^{-\mathrm{i}H_0 t}$ commute, so x_ψ^2 is independent of V.

Integrating now with respect to μ,

$$\begin{aligned} f_\psi(\varepsilon,t) &= \frac{1}{c}\frac{1}{\sqrt{2\,\varepsilon}}\lim_{N\to\infty}\int_{-N}^{N} \mathrm{e}^{\mathrm{i}\lambda t}\,\overline{F\psi(\lambda)}\,\mathcal{F}\Big(\mathrm{e}^{-\left(\frac{\lambda-\mu}{c}\right)^2\frac{1}{4\varepsilon}}\,F\psi(\mu)\Big)(t)\,\mathrm{d}\lambda \\ &= \frac{1}{\sqrt{2\,\pi}\,c}\frac{1}{\sqrt{2\,\varepsilon}}\lim_{N\to\infty}\int_{-N}^{N} \mathrm{e}^{\mathrm{i}\lambda t}\,\overline{F\psi(\lambda)}\Big(\mathcal{F}\,\mathrm{e}^{-\left(\frac{\lambda-\mu}{c}\right)^2\frac{1}{4\varepsilon}}*\mathcal{F}F\psi(\mu)\Big)(t)\,\mathrm{d}\lambda \\ &= \frac{1}{\sqrt{2\,\pi}}\lim_{N\to\infty}\int_{-N}^{N} \mathrm{e}^{\mathrm{i}\lambda t}\,\overline{F\psi(\lambda)}\int \mathrm{e}^{-\mathrm{i}\lambda(t-s)}\,\mathrm{e}^{-\varepsilon c^2(t-s)^2}\,(\mathcal{F}F\psi)(s)\,\mathrm{d}s\,\mathrm{d}\lambda. \end{aligned}$$

Again by Fubini's theorem we may interchange the integrals and this leads us to

$$\begin{aligned} f_\psi(\varepsilon,t) &= \frac{1}{\sqrt{2\,\pi}}\int \overline{\mathrm{e}^{-\mathrm{i}\lambda s}\,F\psi(\lambda)}\,(\mathcal{F}F\psi)(s)\,\mathrm{e}^{-\varepsilon c^2(t-s)^2}\,\mathrm{d}\lambda\,\mathrm{d}s \\ &= \int |(\mathcal{F}F\psi)(s)|^2\,\mathrm{e}^{-\varepsilon c^2(t-s)^2}\,\mathrm{d}s, \quad \text{for } \psi\in P_1\,\mathcal{H}\cup P_2\,\mathcal{H}. \end{aligned}$$

We now compute

$$\begin{aligned} \lim_{\varepsilon\to 0_+} -\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\,f_\psi(\varepsilon,t) &= \lim_{\varepsilon\to 0_+} c^2\int (t-s)^2\,|(\mathcal{F}F\psi)(s)|^2\,\mathrm{e}^{-\varepsilon c^2(t-s)^2}\,\mathrm{d}s \\ &= c^2\int (t-s)^2\,|(\mathcal{F}F\psi)(s)|^2\,\mathrm{d}s, \quad \text{for } \psi\in P_1\,\mathcal{H}\cup P_2\,\mathcal{H}. \end{aligned}$$

Using that

$$(F\psi)(\lambda)=\begin{cases} \sqrt{c}\,\mathcal{F}\left(\mathrm{e}^{\frac{\mathrm{i}}{c}q(c\,\cdot)}\,\psi(c\,\cdot)\right)(\lambda) & \text{a.e., for } \psi\in P_1\,\mathcal{H}, \\ \sqrt{c}\,\mathcal{F}\left(\mathrm{e}^{-\frac{\mathrm{i}}{c}q(-c\,\cdot)}\,\psi(-c\,\cdot)\right)(\lambda) & \text{a.e., for } \psi\in P_2\,\mathcal{H}, \end{cases}$$

and hence

$$(\mathcal{F}F\psi)(s)=\begin{cases} \sqrt{c}\,\mathrm{e}^{\frac{\mathrm{i}}{c}q(-c\,s)}\,\psi(-c\,s) & \text{a.e., for } \psi\in P_1\,\mathcal{H}, \\ \sqrt{c}\,\mathrm{e}^{-\frac{\mathrm{i}}{c}q(c\,s)}\,\psi(c\,s) & \text{a.e., for } \psi\in P_2\,\mathcal{H}, \end{cases}$$

we arrive at

$$\langle\psi(x,t),x^2\,\psi(x,t)\rangle=\begin{cases} c^2\,t^2\,\|\psi\|^2+2\,c\,t\,\langle\psi(x),x\,\psi(x)\rangle+\langle\psi(x),x^2\,\psi(x)\rangle & \text{for } \psi\in P_1\,\mathcal{H}, \\ c^2\,t^2\,\|\psi\|^2-2\,c\,t\,\langle\psi(x),x\,\psi(x)\rangle+\langle\psi(x),x^2\,\psi(x)\rangle & \text{for } \psi\in P_2\,\mathcal{H}. \end{cases}$$

We obtain the desired identity for a general $\psi=P_1\,\psi\oplus P_2\,\psi\in\mathcal{H}$ simply adding up the previous results for $P_1\ \psi$ and $P_2\ \psi$, because the time evolution and the multiplication by the identity operators leave $P_1\,\mathcal{H}$ and $P_2\,\mathcal{H}$ invariant. $\square$

APPENDIX A. SOME USEFUL RESULTS

This section contains important results we use in this text, often without any further reference.

A.1. Spectral theory of self-adjoint operators.

This is mainly a summary of [Wei80, §7.2-§7.4]. We refer to this book for the proofs and further reading. Along this section $\mathcal{H}$ denotes a Hilbert space and H a self-adjoint operator in $\mathcal{H}$.

A family $\{E(t)\}_{t\in\mathbb{R}}$ of orthogonal projections on $\mathcal{H}$ is called a **spectral family** if:

i. $E(s)\leqslant E(t)$ for $s\leqslant t$ (monotonicity),

ii. $E(t+\varepsilon)\xrightarrow{s}E(t)$ for all $t\in\mathbb{R}$, as $\varepsilon\to 0_+$ (continuity from the right)

iii. $E(t)\xrightarrow{s}0$ as $t\to-\infty$ and $E(t)\xrightarrow{s}I$ as $t\to\infty$,

where $\xrightarrow{s}$ denotes the strong limit of operators.

For every $\psi\in\mathcal{H}$, the function $\rho_\psi(t):=\langle E(t)\,\psi,\psi\rangle$ defines a bounded, non-decreasing and right continuous function. A function $f:\mathbb{R}\to\mathbb{C}$ is said to be ***E*-measurable** if it is ρ_ψ-measurable for all $\psi\in\mathcal{H}$. Step functions are E-measurable, and one can define the integral of a step function $u=\sum_{j=1}^n c_j\,\chi(I_j)$ with respect to E by

$$\int u(t)\,\mathrm{d}E(t):=\sum_{j=1}^n c_j\,E(I_j),$$

where $E((a,\,b]):=E(b)-E(a)$, $E((a,\,b)):=E(b_-)-E(a)$, $E([a,\,b]):=E(b)-E(a_-)$ and $E([a,b)):=E(b_-)-E(a_-)$. Approximating with step functions –and with some work– one defines the integral with respect to E of each E-measurable function.

The integral of a real-valued E-measurable function f: $\mathbb{R}\to\mathbb{R}$ is a self-adjoint operator. The following first version of the spectral theorem shows that every self-adjoint operator can be represented in this way.

Theorem A.1. (Spectral theorem, integral version) *For every self-adjoint operator H in a Hilbert space $\mathcal{H}$ there exists exactly one spectral family E for which $H=\int\,t\,\mathrm{d}E(t)$. We say that E is the* ***spectral family*** *of H.*

Another version of the spectral theorem is the multiplication version, which is the infinite-dimensional analogue to the well-known "every hermitian matrix is diagonalizable", or "unitarily equivalent to a diagonal matrix". –Think of the N-dimensional Hilbert space $\mathbb{C}_N$ of functions f: $\{1,\ldots,N\}\to\mathbb{C}$. The multiplication operator by g: $\{1,\ldots,N\}\to\mathbb{C}$ is represented by the diagonal matrix D, with n-th diagonal term $d_{nn}=g(n)$.– In infinite dimensions self-adjoint operators are also unitarily equivalent to multiplications.

Theorem A.2. (Spectral theorem, multiplication version) *Let H be a self-adjoint operator in $\mathcal{H}$. Then there exists a family $\{\rho_\alpha\}_{\alpha\in A}$ of bounded non-zero Borel measures on $\mathbb{R}$ and a unitary operator $U=(U_\alpha)\colon\mathcal{H}\to\bigoplus_{\alpha\in A}L_2(\mathbb{R},\rho_\alpha)$ such that*

$$U\,H\,U^*=\mathrm{Id},$$

where Id *denotes the operator of multiplication by the identity on $\bigoplus_{\alpha\in A}L_2(\mathbb{R},\rho_\alpha)$. The cardinality of A is at most the dimension of $\mathcal{H}$, and for the spectral family E of H we have $U\,E(t)\,U^*=\chi_{(-\infty,t]}$. We call this a* ***spectral representation*** *of H. In contrast to the spectral family, a spectral representation is not unique.*

Let E be a spectral family on $\mathcal{H}$. A subset $M\subset\mathbb{R}$ is said to be ***E*-measurable** if its characteristic function $\chi(M)$ is E-measurable. Extending the definition of $E(I)$ for an interval $I\subset\mathbb{R}$, we set $E(M):=\int\,\chi(M)(t)\,\mathrm{d}E(t)$. The operators $E(M)$ are orthogonal projections and are called **spectral projections**.

Theorem A.3. *Let H be a self-adjoint operator in $\mathcal{H}$ and let E be its spectral family. The following statements are equivalent:*

i. $\lambda \in \sigma(H)$.

ii. *There exists a sequence* $\psi_n \in \mathcal{D}(H)$ *with* $\|\psi_n\| = 1$ *such that* $\|(H - \lambda)\, \psi_n\| \to 0$ *as* $n \to \infty$.

iii. $E(\lambda - \varepsilon, \lambda + \varepsilon) \neq 0$ *for all* $\varepsilon > 0$.

The equivalence (i)⇔(ii) is usually known as **Weyl's criterion**.

A.2. Hilbert-Schmidt operators.

Let $\mathcal{H}$ be a separable Hilbert space and $\{\varphi_n\}_{n=1}^{\infty}$ an orthonormal basis. Let A be a bounded positive operator in $\mathcal{H}$. The **trace** of A is defined as $\operatorname{tr} A := \sum_{n=1}^{\infty} \langle \varphi_n, A\varphi_n \rangle$ and is independent of the choice of $\{\varphi_n\}$. It holds [RS80, Theorem VI.18] that

i. $\operatorname{tr}(U A U^*) = \operatorname{tr} A$, for any unitary operator U.

The trace allows the definition of Banach spaces of (compact) operators which can be thought as the analogous of the L^p-spaces. For instance, the operators A such that $\operatorname{tr}|A| < \infty$ are called **trace class** operators, and the set of such operators is a Banach space with the norm $\|A\|_1 := \operatorname{tr}|A|$. Here we discuss the analogous of L^2, which is also a Hilbert space, called the space of *Hilbert-Schmidt* operators.

A bounded operator A is **Hilbert-Schmidt** if $\operatorname{tr} A^* A < \infty$. We denote the space of Hilbert-Schmidt operators in $\mathcal{H}$ by $B_2(\mathcal{H})$. Some useful properties of this class of operators are ([RS80, Theorem VI.22]):

i. $B_2(\mathcal{H})$ is a vector space.

ii. If $A \in B_2(\mathcal{H})$ and B is bounded, then $A B \in B_2(\mathcal{H})$ and $B A \in B_2(\mathcal{H})$.

iii. If $A \in B_2(\mathcal{H})$, then $A^* \in B_2(\mathcal{H})$.

iv. $B_2(\mathcal{H})$ with the norm $\|A\|_2 := (\operatorname{tr} A^* A)^{1/2}$ is a Hilbert space.

v. Every $A \in B_2(\mathcal{H})$ is compact, and a compact operator A is in $B_2(\mathcal{H})$ if and only if $\sum_{n=1}^{\infty} \lambda_n^2 < \infty$, where λ_n denote the eigenvalues of A.

For Hilbert-Schmidt operators in an L^2-space we have

Theorem A.4. [RS80, Theorem VI.23] *Let (X, ρ) be a measure space and $\mathcal{H} = L^2(X, \rho)$. A bounded operator A is Hilbert-Schmidt if and only if there exists a function*

$$k \in L^2(X \times X, \mathrm{d}\rho \otimes \mathrm{d}\rho)$$

such that

$$(A\psi)(x) = \int k(x, y)\, \psi(y)\, \mathrm{d}\rho(y).$$

Moreover,

$$\|A\|_2^2 = \int |k(x, y)|^2\, \mathrm{d}\rho(x)\, \mathrm{d}\rho(y).$$

And for Hilbert-Schmidt operators into an L^2-space it holds

Theorem A.5. [Wei80, Theorem 6.12] *Let (X, ρ) be a measure space and $\mathcal{H}$ separable Hilbert space. Let A be an injective operator from $\mathcal{H}$ into $L^2(X, \rho)$. There are equivalent*

i. A is the restriction of a Hilbert-Schmidt operator to $\mathcal{D}(A)$.

ii. There exists a function $v: X \to \mathcal{H}$ such that $\|v(\cdot)\| \in L^2(X, \rho)$ and

$$(A\psi)(x) = \langle v(x), \psi \rangle$$

almost everywhere in X and for all $\psi \in \mathcal{D}(A)$.

iii. There exists a function $f \in L^2(X, \rho)$ such that

$$|A\psi(x)| \leqslant \|\psi\|\, f(x)$$

almost everywhere in X and for all $\psi \in \mathcal{D}(A)$.

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Index

Bibliography

[Ber68] Ju M Berezanskii. *Expansions in Eigenfunctions of Selfadjoint Operators*. Translations of Mathematical Monographs. American Mathematical Society, Oct 1968.

[Che77] P R Chernoff. Schrödinger and Dirac Operators with Singular Potentials and Hyperbolic Equations. *Pacific J. Math.*, 72:361–382, 1977.

[Dav95] E B Davies. *Spectral Theory and Differential Operators*. Cambridge Studies in Advanced Mathematics. Cambridge University Press, 1995.

[DK89] Henrique Dreifus and Abel Klein. A new proof of localization in the Anderson tight binding model. *Commun. Math. Phys.*, 124(2):285–299, Jun 1989.

[FMSS85] J Fröhlich, F Martinelli, E Scoppola and T Spencer. Constructive proof of localization in the Anderson tight binding model. *Commun. Math. Phys.*, 101(1):21–46, Mar 1985.

[GT01] D Gilbarg and N S Trudinger. *Elliptic partial differential equations of second order*, volume 224 of *Grundlehren der Mathematischen Wissenschaften*. Springer, 2nd edition, 2001.

[Ike60] T Ikebe. Eigenfunction expansions associated with the Schrödinger operator and their application to scattering theory. *Arch. Rational Mech. Anal.*, 5:1–34, 1960.

[Kod50] K Kodaira. On ordinary differential equations of any even order and the corresponding eigenfunction expansions. *Amer. J. Math.*, 72:502–544, 1950.

[KS78] V Kovalenko and Yu Semenov. Some problems on expansion in generalized eigenfunctions of the Schrödinger operator with strongly singular potentials. *Russian Math. Surveys*, 33:119–157, 1978.

[KS12] Martin Könenberg and Edgardo Stockmeyer. Localization of two-dimensional massless Dirac fermions in a magnetic quantum dot. *J. Spectr. Theory*, (2):115–146, 2012.

[LL01] Elliott H Lieb and Michael Loss. *Analysis*. Graduate Studies in Mathematics. American Mathematical Society, 2nd edition, 2001.

[MS85] F Martinelli and E Scoppola. Remark on the absence of absolutely continuous spectrum for d-dimensional Schrödinger operators with random potential for large disorder or low energy. *Commun. Math. Phys.*, 97(3):465–471, Sep 1985.

[MS13] Josef Mehringer and Edgardo Stockmeyer. Confinement-deconfinement transitions for two-dimensional Dirac particles. *J. Funct. Anal.*, Press 2013.

[Pas80] L A Pastur. Spectral properties of disordered systems in the one-body approximation. *Commun. Math. Phys.*, 75(2):179–196, Jun 1980.

[Pov55] A Y Povzner. On eigenfunction expansions in terms of scattering solutions. *Dokl. Akad. Nauk SSSR*, 104, 1955.

[PS93] Thomas Poerschke and Günter Stolz. On Eigenfunction Expansions and Scattering Theory. *Math. Z.*, 212:337–357, 1993.

[PSW89] Thomas Poerschke, Günter Stolz and Joachim Weidmann. Expansions in Generalized Eigenfunctions of Selfadjoint Operators. *Math. Z.*, 202:397–408, 1989.

[RS75] Michael Reed and Barry Simon. *Methods of Modern Mathematical Physics II, Fourier Analysis, Self-Adjointness*. Academic Press, 1975.

[RS79] Michael Reed and Barry Simon. *Methods of Modern Mathematical Physics III, Scattering Theory*. Academic Press, 1979.

[RS80] Michael Reed and Barry Simon. *Methods of Modern Mathematical Physics I, Functional Analysis. Revised and enlarged edition*. Academic Press, 1980.

[Sch68] Leonard I Schiff. Quantum Mechanics. McGraw-Hill, 1968.

[Sch10] Karl Michael Schmidt. Spectral Properties of Rotationally Symmetric Massless Dirac Operators. *Lett. Math. Phys.*, 92(3):231–241, Apr 2010.

[Sim82] Barry Simon. Schrödinger Semigroups. *Bull. Amer. Math. Soc.*, 7:447–526, Nov 1982.

[Sim10] Barry Simon. *Trace Ideals and Their Applications*. American Mathematical Soc., Mar 2010.

[Sto89] Günter Stolz. *Entwicklung nach verallgemeinerten Eigenfunktionen von Schrödingeroperatoren*. PhD thesis, Johann Wolfgang Goethe-Universität, Frankfurt am Main, 1989.

[Tha92] Bernd Thaller. *The Dirac Equation*. Springer, 1992.

[Wei80] Joachim Weidmann. *Linear Operators in Hilbert Spaces*. Graduate Texts in Mathematics. Springer, 1980.

[Wei87] Joachim Weidmann. *Spectral Theory of Ordinary Differential Operators*, volume 1258 of *Lecture Notes in Mathematics*. Springer, 1987.

[Wey10] H Weyl. Über gewöhnliche Differentialgleichungen mit Singularitäten und die zugehörigen Entwicklungen willkürlicher Funktionen. *Math. Ann.*, 68:220–269, 1910.