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ASYMMETRIC TRANSPORT IN CONTINUOUS TOPOLOGICAL INSULATORS

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In memory of my beloved grandmother, Tova Rosin

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ABSTRACT

This thesis concerns continuous models for 2-dimensional topological insulators. Such systems are characterized by asymmetric transport along a 1-dimensional curve representing the interface between two insulating materials. The asymmetric transport is quantified by an interface conductivity. In two distinct settings, we derive tractable analytic formulas for this interface conductivity and provide a large class of perturbations under which it is stable. Our theory applies to models of twisted bilayer graphene, low-energy superconductors, and relativistic electrons (possibly subject to a magnetic field) described by an appropriate Dirac operator, among others.

Our second main focus is numerical approximations of the above systems. We define a modified interface conductivity on a box with periodic boundary conditions, and show that it is stable and converges rapidly to its infinite-space analogue as the size of the box goes to infinity. We illustrate with several examples that one can restrict a topological insulator to a large and discrete torus to obtain accurate numerical evaluations of the conductivity. Numerical techniques that do not require periodic truncation are also implemented and analyzed. We derive a novel integral equation for the time-harmonic Klein-Gordon equation with appropriate jump conditions along a one-dimensional interface. We implement a fast multipole and sweeping-accelerated iterative algorithm for solving the integral equations, and demonstrate numerically the fast convergence of this method. Several numerical examples of solutions and scattering effects illustrate our theory.

CHAPTER 1

INTRODUCTION

When two insulating materials are brought next to each other, the resulting system may admit edge modes and exhibit a robust and asymmetric transport along the interface. Mathematically, this phenomenon is most often explained by a topological characterization of the two insulators and/or the new material they form. Examples and applications are found in various fields, such as solid state physics, quantum computing, and the geophysical sciences [17, 33, 76, 86, 87]. The focus of this thesis is two-fold: first, to provide a rigorous mathematical analysis of a physical observable that quantifies the above behavior; and second, to perform and analyze numerical approximations of the observable as well as surface waves corresponding to these systems.

In Sections 2 and 3, the physical systems are modeled by (single-particle) Hamiltonians H acting on $\mathcal{H} := L^2(\mathbb{R}^2) \otimes \mathbb{C}^n$ for $n \in \mathbb{N}_+$. We assume that H is a self-adjoint pseudo-differential operator from its domain of definition $\mathcal{D}(H) \subset \mathcal{H}$ to $\mathcal{H}$. We label the spatial coordinates $(x, y) \in \mathbb{R}^2$ and the corresponding dual variables $(\xi, \zeta) \in \mathbb{R}^2$. In the simplest case, the coefficients of (the symbol of) H are constant in (x, y) for $|y| \geq y_0$. Thus H fits the above description with $|y| \geq y_0$ corresponding to the insulating domains, call them $H_\pm$, and the interface of the two materials contained in $|y| < y_0$. Note that a Hamiltonian is called insulating (with respect to an energy interval) if it has a spectral gap (in that interval).

More specifically, in Section 2 below, we will fix $m > 0$ and $-\infty < E_1 < E_2 < \infty$ and consider a large class of Hamiltonians H including those that satisfy

(H1) Let $H = \mathrm{Op}(\sigma)$ with $\sigma \in ES^m_{1,0}$. Suppose there exist symbols $\sigma_\pm \in ES^m_{1,0}$ independent of (x, y) with no spectrum in the open interval (E_1, E_2), such that $\sigma = \sigma_+$ whenever $y \geq y_0$ and $\sigma = \sigma_-$ whenever $y \leq -y_0$, for some $y_0 > 0$.

We refer to Appendix A.1 for notation and definitions. In particular, the symbol class

$ES^m_{1,0}$ is defined below (A.1.4). Moreover, σ is the *symbol* of a Hamiltonian $H = \mathrm{Op}(\sigma)$ written in Weyl quantization (A.1.1) (with $h = 1$), while m is the order of the operator. In most applications, $\sigma(x, y, \xi, \zeta)$ is the matrix-valued symbol of a differential operator of order m.

An important hypothesis is the *ellipticity* condition in the definition of $ES^m_{1,0}$, stating that the singular values of the symbol grow like $|(\xi, \zeta)|^m$ at infinity uniformly in the spatial variables. The second main assumption is that the symbol be independent of position for $|y| \geq y_0$. The slab $-y_0 < y < y_0$ models the transition from the bulk symbol σ_- to the bulk symbol σ_+. The above ellipticity condition implies that H is self-adjoint with domain of definition the standard Hilbert space $\mathcal{H}^m$ in (A.1.3) [20, 56].

Note that we will also use more general hypotheses in Section 2 (allowing for more complicated geometries; see (H0), (H0') and (H1') below), though we now focus on (H1) for ease of exposition.

We now define the following physical observable [7, 10, 17, 37, 40, 41, 77]

$$\sigma_I(H, P, \varphi) := \mathrm{Tr}\, i[H, P]\varphi'(H), \tag{1.0.1}$$

where $\varphi \in \mathfrak{S}(0, 1; E_1, E_2)$ and $P = P(x) \in \mathfrak{S}(0, 1)$. Here, we denote by $\mathfrak{S}(c_1, c_2; \lambda_1, \lambda_2)$ the set of *switch* functions, i.e., smooth real-valued functions f on $\mathbb{R}$ such that $f(x) = c_1$ for $x \leq \lambda_1$ and $f(x) = c_2$ for $x \geq \lambda_2$. The union over $\lambda_1 < \lambda_2$ is denoted by $\mathfrak{S}(c_1, c_2)$.

The conductivity $\sigma_I := \sigma_I(H, P, \varphi)$ is the main object of interest in Section 2. It is a physical observable that can be interpreted as the rate of signal crossing $x_0 \in \mathrm{supp}(P')$ per unit time. Indeed, if $\psi(t) = e^{-itH}\psi_0$ solves the Schrödinger equation, then $\frac{d}{dt}\langle P\rangle_t = \frac{d}{dt}\langle \psi(t), P\psi(t)\rangle = \mathrm{Tr}\ i[H, P][\psi\psi^*](t)$. Replacing the density $\psi\psi^*(t)$ by the stationary mixed state density $\varphi'(H)$ provides the above interpretation to σ_I. It therefore characterizes asymmetric transport along the interface.

The explicit computation of σ_I as the above trace is tractable for Dirac operators [7] and more general operators with sufficiently simple spectral decomposition [10]. In a variety of settings however, σ_I has been shown to equal a difference of bulk topological invariants:

$$2\pi\sigma_I(H, P, \varphi) = I(H_+) - I(H_-),$$

which are often significantly simpler to compute. Such a result is called a bulk-edge or bulk-interface correspondence [7, 10, 37, 40, 42, 49, 68]. The above conductivity has also been related to the (necessarily quantized) index of a Fredholm operator in various contexts; see [7, 10]. In Section 2.4, we extend these results to prove that

$$2\pi\sigma_I(H, P, \varphi) = \mathrm{Index}(\bar{P}U(H)\bar{P}) \tag{1.0.2}$$

for a large class of Hamiltonians including (H1). When H satisfies (H1), the above holds if $\bar{P} = \bar{P}(x)$ is the Heavyside step function, with $P(x) = P \in \mathfrak{S}(0, 1)$ smooth as before. Note that (1.0.2) implies that σ_I is immune to "continuous" perturbations (to be defined in Section 2.4 below), as the right-hand side must be integer-valued. The derivation of (1.0.2) involves a powerful result from [6], which relates the Fredholm index to various traces.

First, however, we directly prove the stability of σ_I without using index theory; see Section 2.1. In Section 2.2, we prove a bulk-interface correspondence for all Hamiltonians satisfying (H1) by deriving an accessible Fedosov-Hörmander formula for σ_I. We next show the usefulness of such a correspondence and compute the conductivity explicitly from the Fedosov-Hörmander formula for a number of models coming from solid state physics [10, 17, 86] and (properly regularized) equatorial waves [10, 33, 48, 79]; see also [15] for an application to compute topological invariants of replica models for Floquet topological insulators. Section 2.4 then generalizes the theory from Sections 2.1–2.3 to junction (rather than interface) models, with applications to materials such as twisted bilayer graphene.

The theory in Section 2 applies to a number of systems of differential equations that appear as low-energy models for many topological insulators and superconductors. However, it does not apply to the magnetic Schrödinger equations that model the integer quantum Hall effect [5, 6, 16], or to partial-differential models with micro-structures [37, 44].

In Section 3, we calculate σ_I and prove its stability in the context of magnetic Dirac equations. Such equations are used in models of graphene subject to external electric and magnetic fields. The magnetic Dirac Hamiltonian is not elliptic and thus the analysis from Section 2 does not apply. Instead, σ_I is related to a spectral flow (see (3.0.5) below), which we calculate explicitly.

The magnetic Dirac Hamiltonian implements three domain walls that induce asymmetric transport. These domain walls correspond to transitions in the magnetic field, electric potential, and a "mass term" across two insulating materials. The existing literature has analyzed separately the roles of a bounded mass term [7, 10] and magnetic field [29] in generating asymmetric transport for Dirac models. To our knowledge, this work is the first to combine the two effects.

The magnetic Dirac Hamiltonian, H, is given by (3.0.2). Its square satisfies $H^2 = D_x^2 + (D_y - A_2(x))^2 + V(x)D_x\sigma_1 + V(x)(D_y - A_2(x))\sigma_2 + R$ for R bounded. The leading-order terms $D_x^2 + (D_y - A_2(x))^2$ are precicely the *Iwatsuka Hamiltonian* analyzed in [35], where there are many results analogous to the ones in this paper. Bulk invariants for magnetic Schrödinger operators are proposed and analyzed in [6, 16]. The distinguishing features of our setting are the additional domain walls m (the mass term) and V (the electric potential), the lack of definiteness of H (the spectrum of H is not bounded above or below), and the fact that H is a first-order matrix valued differential operator (instead of a second-order scalar one). As we will see below, the lack of definiteness perhaps provides the biggest challenge; it will be easy to estimate the absolute value of spectral branches of H, but obtaining the sign of these branches will require more care.

In [28], the interface conductivity is calculated for magnetic Schrödinger Hamiltonians with constant magnetic field and confining potentials. The interface conductivity is induced by the potentials much like an "edge conductivity" would be generated by "hard wall" Dirichlet boundary conditions. A bulk-edge correspondence (involving the edge conductivity) for magnetic Dirac models is proven in [29].

A main result in Section 3 is to derive an explicit expression for $2\pi\sigma_I$ by means of a spectral flow; see Theorems 3.1.1 and 3.2.5 below. We show that $2\pi\sigma_I$ is quantized and (for positive energies and constant m and V) decreases in uniform increments as the strength of the magnetic field increases. This behavior of the interface conductivity resembles the integer quantum Hall effect. Theorem 3.1.1 is a bulk-interface correspondence in that it relates the spectral flow of H to a difference of bulk quantities. The terms in the difference are not expressed as bulk invariants, such as for instance Chern numbers as introduced in [16, 29]. This issue, addressed for non-magnetic Dirac Hamiltonians in [7, 10], is not considered further here. For existing results on the bulk-interface correspondence involving a spectral flow, see also [7, 47].

Section 4 concerns numerical approximations of topological insulators. We consider Hamiltonians H satisfying (H1), and restrict them to a box of size L with periodic boundary conditions. We define a modified interface conductivity (see (4.0.3) below) on the periodic domain, and show that it converges to its infinite space analogue super-algebraically in L^{-1} as $L \to \infty$. We prove stability of the modified conductivity in the same limit, and demonstrate our theoretical results with numerical examples.

The approximate interface conductivity (4.0.3), which is easily estimated computationally, serves as the main spectral object quantifying the topological nature of the asymmetric transport between insulators in a periodic setting. Several works have addressed the computation of bulk topological indices [62, 63, 64, 67, 78], based on the notion of "spectral localizer index", typically determined by the signs of eigenvalues of an appropriate finite dimensional matrix. The numerical index was used recently in [65] to determine numerically the interface along which wave packets may propagate. For an analysis of the propagation of wave packets along curved interfaces in a Dirac model, see [12]. Eigenvalues and edge states for discrete and continuous models are also computed numerically in [83] using a method that avoids artificial Dirichlet boundary conditions by utilizing the resolvent of the Hamiltonian.

In Section 5, we derive novel integral equations for the time-harmonic Klein-Gordon equation in the presence of an interface. Solutions are surface waves that are exponentially localized to the vicinity of the interface, and propagate outward to infinity. The original PDE is inspired by Dirac equations, which are ubiquitous in the analysis of topological insulators (see Section 5.1.2). We analyze the mathematical properties (including well-posedness) of our integral equations in Section 5.2, and present a numerical method for solving them in Section 5.3. Examples of solutions and scattering effects are illustrated in Section 5.4.

Similar models to this one arise, and have been studied in a variety of contexts. For work on the related topic of "leaky quantum graphs" and derivation of similar integral equations, we refer to [43] and references therein. Under the assumption that Γ is a compact perturbation of the flat interface, [43] for instance derives asymptotic expansions for generalized eigenfunctions of the Helmholtz operator and obtains expressions for reflection coefficients in a corresponding scattering theory. Note that our setting places no restriction on the angle between the asymptotic branches of Γ. The point spectrum of elliptic second-order partial differential operators with "singular interactions" along a compact interface has also been analyzed, with an integral formulation in [54]. A Galerkin method for solving it is then proposed there.

Surface waves and plasmon waves also arise naturally in other physical contexts such as the solution of Maxwell's equation in a dielectric medium where the ratio of permittivities approach a negative real number, see [69, 85] and the references therein and [52, 51, 53] for numerical methods. Finally, similar surface-wave preconditioners also referred to as on-surface radiation conditions have been used in other contexts for solving high-frequency scattering problems in acoustics, electromagnetics, and elasticity, see [2, 3, 4, 26, 25, 32, 59] and the references therein. The on-surface radiation conditions are typically used to improve the performance of iterative solvers in complicated geometries and the high-frequency regime and not for the resolution of surface waves inherent to the governing equations.

CHAPTER 2

ELLIPTIC INTERFACE MODELS

2.1 Stability of physical observable

The purpose of this section is to show that $\sigma_I(H, P, \varphi)$ introduced in (1.0.1) is well defined, and prove its stability under perturbations of H, P and φ. The following results are obtained using the theory of pseudo-differential operators (see appendix A) and stability properties of the trace. Similar results are derived in [10, 11] by showing that σ_I is the index of a Fredholm operator, which is known to be invariant under continuous deformations [56]. Here, we do not relate σ_I to any index and instead prove its stability directly, as is done in other contexts in [37, 40, 49, 68].

While the results in this section are significant in their own right, they will also be used to prove Theorem 2.2.1 below (one of the main results of the paper). The following stability properties of σ_I show that the latter can be computed in the semi-classical limit (see Theorem 2.1.11). This allows for a Fedosov-Hörmander formula (2.2.7) for the conductivity, which is the subject of section 2.2.

To prove that σ_I is stable, it will be useful to define the following class of pseudo-differential operators, where we fix $\tilde{E}_1 < \tilde{E}_2$, and let $\Phi \in \mathcal{C}_c^\infty(\mathbb{R})$ such that $\Phi \equiv 1$ in $[\tilde{E}_1, \tilde{E}_2]$.

(H0) Let $H = \mathrm{Op}(\sigma)$, such that $\sigma \in ES^m_{1,0}$ and $\Phi(H) \in \mathrm{Op}(S(\langle y, \xi, \zeta\rangle^{-\infty}))$.

By Proposition A.3.1, any H satisfying (H0) is self-adjoint with domain of definition $\mathcal{D}(H) = \mathcal{H}^m$. Moreover, $(z - H)^{-1} \in \mathrm{Op}(S(\langle \xi, \zeta\rangle^{-m}))$ with symbolic bounds that blow up algebraically as $\Im z \to 0$. For any $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$ and $s \in \mathbb{N}$, we have $\psi(H) = (i - H)^{-s}\phi_s(H)$ for some $\phi_s \in \mathcal{C}_c^\infty(\mathbb{R})$. Using the Helffer-Sjöstrand formula and composition calculus, this implies that $\psi(H) \in \mathrm{Op}(S(\langle \xi, \zeta\rangle^{-\infty}))$ for every $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$. If, in particular,

$\psi \in \mathcal{C}_c^\infty(\tilde{E}_1, \tilde{E}_2)$, then (H0) and the composition calculus imply that $\psi(H) = \psi(H)\Phi(H) \in \mathrm{Op}(S(\langle y, \xi, \zeta\rangle^{-\infty}))$.

Note that if $\Phi \in \mathcal{C}_c^\infty(E_1, E_2)$, then any operator H satisfying (H1) must also satisfy (H0); see Proposition 2.1.10 below. However, all of the results before Proposition 2.1.10 will assume only that H satisfies (H0).

We first show that $\sigma_I(H, P, \varphi)$ is well defined.

Lemma 2.1.1. *Suppose H satisfies (H0), and let $P(x) = P \in \mathfrak{S}(0,1)$ and $\varphi \in \mathfrak{S}(0,1; \tilde{E}_1, \tilde{E}_2)$. Then $[H, P]\varphi'(H)$ is trace-class. If $\psi \in \mathcal{C}_c^\infty(\tilde{E}_1, \tilde{E}_2)$, then $q(H)[\psi(H), P]$ is trace-class for any polynomial q.*

Proof. Recall that $\varphi' \in \mathcal{C}_c^\infty(\tilde{E}_1, \tilde{E}_2)$, and hence $\varphi'(H) \in \mathrm{Op}(S(\langle y, \xi, \zeta\rangle^{-\infty}))$. Since $[H, P] = (1-P)HP - PH(1-P) \in \mathrm{Op}(S(\langle x\rangle^{-\infty}\langle y, \xi, \zeta\rangle^{m}))$, the composition calculus implies that $[H, P]\varphi'(H)$ is trace-class.

Now if $\psi \in \mathcal{C}_c^\infty(\tilde{E}_1, \tilde{E}_2)$, then $\psi(H) \in \mathrm{Op}(S(\langle y, \xi, \zeta\rangle^{-\infty}))$, and thus $[\psi(H), P] = (1 - P)\psi(H)P - P\psi(H)(1-P) \in \mathrm{Op}(S(\langle x, y, \xi, \zeta\rangle^{-\infty}))$ by the composition calculus. Since $q(H) \in \mathrm{Op}(S(\langle \xi, \zeta\rangle^{km}))$ for some $k \in \mathbb{N}$, it follows that

$$q(H)[\psi(H), P] \in \mathrm{Op}(S(\langle x, y, \xi, \zeta\rangle^{-\infty}))$$

is trace-class. □

Our next result shows that the trace in (1.0.1) is not modified after regularization of the commutator.

Lemma 2.1.2. *Let $P(x) = P \in \mathfrak{S}(0,1)$ and $\varphi \in \mathfrak{S}(0,1; \tilde{E}_1, \tilde{E}_2)$. Let S be any open interval containing* $\operatorname{supp}\varphi'$, *and let $\Psi \in \mathcal{C}_c^\infty(\mathbb{R})$ such that $\Psi(\lambda) = \lambda$ in S. Then given any self-adjoint H for which $[H, P]\varphi'(H)$ is trace-class, it follows that $[\Psi(H), P]\varphi'(H)$ is trace-class, with*

$$\sigma_I(H, P, \varphi) = \operatorname{Tr} i[\Psi(H), P]\varphi'(H). \tag{2.1.1}$$

By Lemma 2.1.1, we know that Lemma 2.1.2 applies to any H satisfying (H0).

Proof. Using the Helffer-Sjöstrand formula, we write

$$\begin{aligned}[\Psi(H), P] &= \Big[-\frac{1}{\pi}\int_{\mathbb{C}} \bar\partial\tilde\Psi(z)(z-H)^{-1}d^2z, P\Big] \\ &= -\frac{1}{\pi}\int_{\mathbb{C}} \bar\partial\tilde\Psi(z)(z-H)^{-1}[H,P](z-H)^{-1}d^2z,\end{aligned}$$

which implies that

$$[\Psi(H), P]\varphi'(H) = -\frac{1}{\pi}\int_{\mathbb{C}} \bar\partial\tilde\Psi(z)(z-H)^{-1}[H,P]\varphi'(H)(z-H)^{-1}d^2z.$$

Since $\big\|(z-H)^{-1}\big\| \le |\Im z|^{-1}$ with $\bar\partial\tilde\Psi \in \mathcal{C}_c^\infty(\mathbb{C})$ and $|\bar\partial\tilde\Psi|(z) \le C|\Im z|^2$, the assumption that $[H,P]\varphi'(H)$ is trace-class implies that $[\Psi(H),P]\varphi'(H)$ must be trace-class as well.

Let $\Phi_0, \Phi_{00} \in \mathcal{C}_c^\infty(\mathbb{R})$ such that $\varphi' = \varphi'\Phi_0 = \varphi'\Phi_{00}$ and $\Phi_0 = \Phi_0\Phi_{00}$, with $\Psi\Phi_{00} = \lambda\Phi_{00}$. Below, we use the shorthand $f := f(H)$ for all compactly supported functions f. It follows from cyclicity of the trace [57] that

$$\begin{aligned}\mathrm{Tr}[H,P]\varphi' &= \mathrm{Tr}[H,P]\varphi'\Phi_0 = \mathrm{Tr}\,\Phi_0[H,P]\varphi' = \mathrm{Tr}\,\Phi_0(\Phi_{00}HP - PH\Phi_{00})\varphi' \\ &= \mathrm{Tr}\,\Phi_0(\Phi_{00}\Psi P - P\Psi\Phi_{00})\varphi' = \mathrm{Tr}\,\Phi_0[\Psi,P]\varphi' = \mathrm{Tr}[\Psi,P]\varphi',\end{aligned}$$

and the proof is complete. $\square$

We now show that the conductivity is independent of $\varphi \in \mathfrak{S}(0,1;\tilde E_1,\tilde E_2)$.

Proposition 2.1.3. *Suppose H satisfies (H0), and let $P(x) = P \in \mathfrak{S}(0,1)$ and $\varphi_1,\varphi_2 \in \mathfrak{S}(0,1;\tilde E_1,\tilde E_2)$. Then*

$$\sigma_I(H,P,\varphi_1) = \sigma_I(H,P,\varphi_2).$$

Proof. It suffices to show that $\operatorname{Tr} i[H,P]\phi'(H) = 0$ for all $\phi \in \mathcal{C}_c^\infty(\tilde{E}_1, \tilde{E}_2)$. Let $\psi \in \mathcal{C}_c^\infty(\tilde{E}_1, \tilde{E}_2)$ such that $\psi(\lambda) = \lambda$ for all λ in some open interval containing $\operatorname{supp}(\phi)$. It follows that

$$\begin{aligned}
\operatorname{Tr}[H,P]\phi'(H) = \operatorname{Tr}[\psi(H),P]\phi'(\psi(H)) &= \operatorname{Tr}\Big(-\frac{1}{\pi}[\psi(H),P]\int_{\mathbb{C}} \bar{\partial}\tilde{\phi}'(z)(z-\psi(H))^{-1}d^2z\Big) \\
&= \operatorname{Tr}\Big(-\frac{1}{\pi}[\psi(H),P]\int_{\mathbb{C}} \bar{\partial}\tilde{\phi}(z)(z-\psi(H))^{-2}d^2z\Big) \\
&= \operatorname{Tr}\Big(-\frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\phi}(z)(z-\psi(H))^{-1}[\psi(H),P](z-\psi(H))^{-1}d^2z\Big) \\
&= \operatorname{Tr}\Big[-\frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\phi}(z)(z-\psi(H))^{-1}d^2z, P\Big] = \operatorname{Tr}[\phi(H),P],
\end{aligned}$$

where we have used Lemma 2.1.2 to justify the first equality, the Helffer-Sjöstrand formula for the second and last equalities, integration by parts in ∂ for the third equality, cyclicity of the trace for the fourth equality, and the identity $[(z-A)^{-1},B] = (z-A)^{-1}[A,B](z-A)^{-1}$ for the fifth equality.

Now, let $P_1, P_2 \in \mathfrak{S}(0,1)$ with $P_j = P_j(x)$ such that $PP_1 = P$ and $(1-P)(1-P_2) = 1-P$. Then

$$\begin{aligned}
\operatorname{Tr}[\phi(H),P] &= \operatorname{Tr}((1-P)\phi(H)P - P\phi(H)(1-P)) = \operatorname{Tr}(1-P)\phi(H)P - \operatorname{Tr}P\phi(H)(1-P) \\
&= \operatorname{Tr}(1-P)\phi(H)PP_1 - \operatorname{Tr}P\phi(H)(1-P)(1-P_2) \\
&= \operatorname{Tr}P_1(1-P)\phi(H)P - \operatorname{Tr}(1-P_2)P\phi(H)(1-P) \\
&= \operatorname{Tr}PP_1(1-P)\phi(H) - \operatorname{Tr}(1-P)(1-P_2)P\phi(H) \\
&= \operatorname{Tr}P(1-P)\phi(H) - \operatorname{Tr}(1-P)P\phi(H) = 0,
\end{aligned}$$

and the proof is complete. $\square$

We now prove the stability of the trace with respect to changes in the domain wall P.

Proposition 2.1.4. *Suppose H satisfies (H0), $\varphi \in \mathfrak{S}(0,1;\tilde{E}_1,\tilde{E}_2)$, and $P_1, P_2 \in \mathfrak{S}(0,1)$*

with $P_j = P_j(x)$*. Then*

$$\sigma_I(H, P_1, \varphi) = \sigma_I(H, P_2, \varphi).$$

Proof. Using Lemma 2.1.2, we have

$$\sigma_I(H, P_2, \varphi) - \sigma_I(H, P_1, \varphi) = \operatorname{Tr} i[\Psi(H), P_2 - P_1]\varphi'(H).$$

Since $P_2 - P_1 \in \langle x\rangle^{-\infty}$, the assumption (H0) implies that $(P_2 - P_1)\varphi'(H)$ is trace-class. Therefore,

$$\begin{aligned}\operatorname{Tr} i[\Psi(H), P_2 - P_1]\varphi'(H) &= \operatorname{Tr} i\Psi(H)(P_2 - P_1)\varphi'(H) - \operatorname{Tr} i(P_2 - P_1)\Psi(H)\varphi'(H) \\ &= \operatorname{Tr} i(P_2 - P_1)\varphi'(H)\Psi(H) - \operatorname{Tr} i(P_2 - P_1)\Psi(H)\varphi'(H) = 0,\end{aligned}$$

where we have used cyclicity of the trace to justify the second equality, and the fact that $[\varphi'(H), \Psi(H)] = 0$ for the last equality. $\square$

We have shown that if H satisfies (H0), then $\sigma_I(H, P, \varphi)$ is independent of $P(x) = P \in \mathfrak{S}(0, 1)$ and $\varphi \in \mathfrak{S}(0, 1; E_1, E_2)$. Now we want to analyze the stability of $\sigma_I(H, P, \varphi)$ with respect to perturbations of H. For W a symmetric linear operator (with various additional assumptions in the results below), let

$$H^{(\mu)} = H + \mu W \quad \text{for} \quad \mu \in [0, 1].$$

We begin by introducing a class of appropriately decaying perturbations under which the interface conductivity is stable.

Theorem 2.1.5. *Suppose* H *satisfies (H0),* $P(x) = P \in \mathfrak{S}(0, 1)$ *and* $\varphi \in \mathfrak{S}(0, 1; \tilde{E}_1, \tilde{E}_2)$*. Assume that* W *is symmetric with* $W \in \operatorname{Op}(S^m_{1,0} \cap S(\langle x, y\rangle^{-\delta}))$ *for some* $\delta > 0$*. If* $H^{(1)}$

satisfies (H0), then $\sigma_I(H^{(1)}, P, \varphi) = \sigma_I(H, P, \varphi)$.

Proof. The assumption that $H^{(1)}$ satisfies (H0) implies $\sigma_I(H^{(1)}, P, \varphi)$ is well defined (see Lemma 2.1.1), with

$$\sigma_I(H^{(1)}, P, \varphi) - \sigma_I(H, P, \varphi) = \\ \operatorname{Tr} i[\Psi(H^{(1)}), P](\varphi'(H^{(1)}) - \varphi'(H)) + \operatorname{Tr} i[\Psi(H^{(1)}) - \Psi(H), P]\varphi'(H)$$

by Lemma 2.1.2. Using cyclicity of the trace as in the proof of Proposition 2.1.3, we find that

$$\operatorname{Tr} i[\Psi(H^{(1)}) - \Psi(H), P]\varphi'(H) = -\operatorname{Tr} i[\varphi'(H), P](\Psi(H^{(1)}) - \Psi(H)).$$

Thus by Proposition 2.1.4, it suffices to show that $\operatorname{Tr}[A, P_{x_0}]B \to 0$ as $x_0 \to \infty$ for $A \in \{\Psi(H^{(1)}), \varphi'(H)\}$ and $B \in \{\varphi'(H^{(1)}) - \varphi'(H), \Psi(H^{(1)}) - \Psi(H)\}$, where $P_{x_0}(x) := P(x - x_0)$.

Fix $\varepsilon > 0$. For any $\phi \in \mathcal{C}_c^\infty(\tilde{E}_1, \tilde{E}_2)$, the Helffer-Sjöstrand formula implies that

$$\phi(H^{(1)}) - \phi(H) = \frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\phi}(z)(z - H^{(1)})^{-1}W(z - H)^{-1}d^2z.$$

Propositions A.2.1 and A.3.1 (together with the rapid decay of $\bar{\partial}\tilde{\phi}$ near the real axis) then imply that

$$\phi(H^{(1)}) - \phi(H) \in \operatorname{Op}(S(\langle x, y\rangle^{-\delta}\langle \xi, \zeta\rangle^{-m})) \subset \operatorname{Op}(S(\langle x, y, \xi, \zeta\rangle^{-\delta})), \tag{2.1.2}$$

where we have assumed without loss of generality that $\delta < m$. Thus $B \in \operatorname{Op}(S(\langle x, y, \xi, \zeta\rangle^{-\delta}))$, so there exist $b_0 \in \mathcal{C}_c^\infty(\mathbb{R}^4)$ and $b_1 \in S(1)$ as small as necessary such that $B = B_0 + B_1$ with $B_j := \operatorname{Op}(b_j)$ and $\|B_1\| < \varepsilon$. Writing $[A, P_{x_0}] = (1 - P_{x_0})AP_{x_0} - P_{x_0}A(1 - P_{x_0})$, Lemma 2.1.6 and the composition calculus imply that $[A, P_{x_0}] \in \operatorname{Op}(S(\langle x - x_0, y, \xi, \zeta\rangle^{-\infty}))$ uniformly in

x_0. We conclude that $\|[A, P_{x_0}]\|_1 \leq C$ uniformly in x_0, hence $\limsup_{x_0 \to \infty} \|[A, P_{x_0}]B_1\|_1 < C\varepsilon$. Moreover, the decay of b_0 implies that

$$\|[A, P_{x_0}]B_0\|_1 \leq C \int_{\mathbb{R}^4} \langle x - x_0, y, \xi, \zeta \rangle^{-5} \langle x, y, \xi, \zeta \rangle^{-5} dx dy d\xi d\zeta \longrightarrow 0$$

as $x_0 \to \infty$. We have thus shown that

$$\limsup_{x_0 \to \infty} \|[A, P_{x_0}]B\|_1 \leq \limsup_{x_0 \to \infty} \|[A, P_{x_0}]B_0\|_1 + \limsup_{x_0 \to \infty} \|[A, P_{x_0}]B_1\|_1 < C\varepsilon.$$

Since ε was arbitrary, the proof is complete. $\square$

Next, we introduce a class of relatively compact perturbations W for which the symbols of compactly supported functionals of $H^{(1)}$ decay rapidly in $\langle y, \xi, \zeta \rangle$.

Lemma 2.1.6. *Suppose H satisfies (H0), and let W be a symmetric pseudo-differential operator such that $W \in \mathrm{Op}(S^m_{1,0} \cap S(\langle \xi, \zeta \rangle^{m-\delta} \langle x, y \rangle^{-\delta}))$ for some $\delta > 0$. Then $H^{(1)} \in \mathrm{Op}(ES^m_{1,0})$ is self-adjoint with domain of definition $\mathcal{H}^m$, and $\phi(H^{(1)}) \in \mathrm{Op}(S(\langle y, \xi, \zeta \rangle^{-\infty}))$ for any $\phi \in \mathcal{C}^\infty_c(\tilde{E}_1, \tilde{E}_2)$.*

Proof. That $H^{(1)} \in \mathrm{Op}(ES^m_{1,0})$ follows immediately from ellipticity of H and the decay of W. By Proposition A.3.1, this means $H^{(1)}$ is self-adjoint with domain of definition $\mathcal{H}^m$. Moreover, $(z - H^{(1)})^{-1} \in \mathrm{Op}(S(\langle \xi, \zeta \rangle^{-m}))$ for all $\Im z \neq 0$, with symbolic bounds blowing up at worst algebraically as $\Im z \to 0$ (see Proposition A.3.1).

Let $\phi, \phi_0 \in \mathcal{C}^\infty_c(\tilde{E}_1, \tilde{E}_2)$ such that $\phi\phi_0 = \phi$, and define $\Theta := \phi(H^{(1)}) - \phi(H)$ and $\Theta_0 := \phi_0(H^{(1)}) - \phi_0(H)$. Then $\Theta = \Theta\Theta_0 + \phi(H)\Theta_0 + \Theta\phi_0(H)$, and hence

$$\Theta(1 - \Theta_0) = \phi(H)\Theta_0 + \Theta\phi_0(H).$$

By (2.1.2), we have $\Theta, \Theta_0 \in \mathrm{Op}(S(\langle x, y, \xi, \zeta \rangle^{-\delta}))$. Thus there exist $\theta_{00} \in \mathcal{C}^\infty_c(\mathbb{R}^4)$ and $\theta_{01} \in S(1)$ as small as necessary such that $\Theta_{00} = \mathrm{Op}(\theta_{00})$, $\Theta_{01} = \mathrm{Op}(\theta_{01})$ with $\|\Theta_{01}\| < 1$

(see Proposition A.2.2), and $\Theta_0 = \Theta_{00} + \Theta_{01}$. Since $\phi(H), \phi_0(H) \in \mathrm{Op}(S(\langle y, \xi, \zeta\rangle^{-\infty}))$ by assumption on H, it follows that

$$\Theta(1 - \Theta_{01}) = \Theta(1 - \Theta_0) + \Theta\Theta_{00} \in \mathrm{Op}(S(\langle y, \xi, \zeta\rangle^{-\infty})),$$

hence

$$\Theta = (\Theta(1 - \Theta_0) + \Theta\Theta_{00})(1 - \Theta_{01})^{-1} \in \mathrm{Op}(S(\langle y, \xi, \zeta\rangle^{-\infty})).$$

We conclude that $\phi(H^{(1)}) = \phi(H) + \Theta \in \mathrm{Op}(S(\langle y, \xi, \zeta\rangle^{-\infty}))$, and the proof is complete. $\square$

We now show that the interface conductivity is stable with respect to this class of relatively compact perturbations W.

Theorem 2.1.7. *Suppose H satisfies (H0), $P(x) = P \in \mathfrak{S}(0, 1)$ and $\varphi \in \mathfrak{S}(0, 1; \tilde{E}_1, \tilde{E}_2)$. If W is symmetric with $W \in \mathrm{Op}(S^m_{1,0} \cap S(\langle \xi, \zeta\rangle^{m-\delta}\langle x, y\rangle^{-\delta}))$ for some $\delta > 0$, then*

$$\sigma_I(H^{(1)}, P, \varphi) = \sigma_I(H, P, \varphi).$$

Proof. Fix $\phi \in \mathcal{C}^\infty_c(\tilde{E}_1, \tilde{E}_2)$ such that $\phi \equiv 1$ in some open interval containing $\mathrm{supp}(\varphi')$. Lemma 2.1.6 then implies that $H^{(1)}$ satisfies (H0), with Φ replaced by ϕ. The result then follows from Theorem 2.1.5. $\square$

Next, we derive a stability result that no longer requires the perturbation to be relatively compact. We will instead assume that W is relatively bounded with respect to H, and require that W be "sufficiently small."

Theorem 2.1.8. *Suppose H satisfies (H0), $P(x) = P \in \mathfrak{S}(0, 1)$ and $\varphi \in \mathfrak{S}(0, 1; \tilde{E}_1, \tilde{E}_2)$. If W is symmetric with $W \in \mathrm{Op}(S^m_{1,0})$, then $\sigma_I(H^{(\mu)}, P, \varphi) = \sigma_I(H, P, \varphi)$ for all $\mu > 0$ sufficiently small.*

In the proof below, we will be analyzing operators $A = \mathrm{Op}(a)$ that depend on the parameter μ. For $\mathfrak{m} : \mathbb{R}^4 \to [0, \infty)$ an order function, we will write $A \in \mathrm{Op}(\mu S(\mathfrak{m}))$ to mean that $a \in S(\mathfrak{m})$ for all μ, with $|\partial^\alpha a| \le C_\alpha \mu \mathfrak{m}$ uniformly in μ.

Proof. Since $H \in \mathrm{Op}(ES^m_{1,0})$ and W is symmetric, it follows that $H^{(\mu)} \in \mathrm{Op}(ES^m_{1,0})$ is self-adjoint (with domain of definition $\mathcal{H}^m$) whenever $\mu > 0$ is sufficiently small.

Let $\phi, \phi_0 \in \mathcal{C}_c^\infty(E_1, E_2)$ such that $\phi\phi_0 = \phi$. Following the proof of Lemma 2.1.6, we define $\Theta := \phi(H^{(\mu)}) - \phi(H)$ and $\Theta_0 := \phi_0(H^{(\mu)}) - \phi_0(H)$, and verify that

$$\Theta(1 - \Theta_0) = \phi(H)\Theta_0 + \Theta\phi_0(H).$$

The Helffer-Sjöstrand formula implies that

$$\Theta_0 = -\frac{\mu}{\pi} \int_{\mathbb{C}} \bar{\partial}\tilde{\phi_0}(z)(z - H^{(\mu)})^{-1} W (z - H)^{-1} d^2 z.$$

By Propositions A.2.1 and A.3.2, this means $\Theta_0 \in \mathrm{Op}(\mu S(\langle \xi, \zeta\rangle^{-m}))$. It follows that $(1 - \Theta_0)^{-1} \in \mathrm{Op}(S(1))$ whenever $\mu > 0$ is sufficiently small, hence

$$\Theta = (\phi(H)\Theta_0 + \Theta\phi_0(H))(1 - \Theta_0)^{-1} \in \mathrm{Op}(S(\langle y, \xi, \zeta\rangle^{-\infty}))$$

by (H0). We conclude that $\phi(H^{(\mu)}) = \phi(H) + \Theta \in \mathrm{Op}(S(\langle y, \xi, \zeta\rangle^{-\infty}))$. Since ϕ was arbitrary, this means $\sigma_I(H^{(\mu)}, P, \varphi)$ is well defined whenever $\mu > 0$ is small enough.

Let $\chi \in \mathfrak{S}(1, 0; 1, 2)$ be monotonically non-increasing, and define

$$\chi_\varepsilon(x, y, \xi, \zeta) := \chi(\varepsilon|(x, y, \xi, \zeta)|)$$

and $H^{(\mu,\varepsilon)} := \mathrm{Op}(\sigma + \mu\chi_\varepsilon w)$ for $\varepsilon \in (0, 1]$. Since $\chi_\varepsilon w \in S(\langle x, y, \xi, \zeta\rangle^{-\infty})$, Theorem 2.1.7

implies that

$$\sigma_I(H^{(\mu,\varepsilon)}, P, \varphi) = \sigma_I(H, P, \varphi), \qquad \varepsilon \in (0,1].$$

It remains to show that $\sigma_I(H^{(\mu,\varepsilon)}, P, \varphi) - \sigma_I(H^{(\mu)}, P, \varphi) \to 0$ as $\varepsilon \downarrow 0$. In order to do this, we will first need symbolic bounds that are uniform in μ and ε.

For any multi-index α and any $p > 0$, we have $|\partial^\alpha \chi_\varepsilon|(x, y, \xi, \zeta) \le C_{\alpha,p}\varepsilon^{|\alpha|}\langle \varepsilon x, \varepsilon y, \varepsilon\xi, \varepsilon\zeta\rangle^{-p}$ uniformly in ε. In particular, this means

$$|\partial^\alpha \chi_\varepsilon|(x, y, \xi, \zeta) \le C_{\alpha,|\alpha|}\varepsilon^{|\alpha|}\langle \varepsilon x, \varepsilon y, \varepsilon\xi, \varepsilon\zeta\rangle^{-|\alpha|} \le C_{\alpha,|\alpha|}\langle x, y, \xi, \zeta\rangle^{-|\alpha|}, \qquad \varepsilon \in (0,1].$$

By definition, $\mathrm{Op}(w) := W$ satisfies $|\partial^{\beta_1}_{x,y}\partial^{\beta_2}_{\xi,\zeta} w|(x, y, \xi, \zeta) \le C_\beta \langle \xi, \zeta\rangle^{m-|\beta_2|}$ for any multi-index $\beta = (\beta_1, \beta_2)$. It follows that

$$|\partial^\alpha \chi_\varepsilon \partial^\beta w|(x, y, \xi, \zeta) \le C_{\alpha,\beta}\langle x, y, \xi, \zeta\rangle^{-|\alpha|}\langle \xi, \zeta\rangle^{m-|\beta_2|} \le C_{\alpha,\beta}\langle \xi, \zeta\rangle^{m-|\alpha_2|-|\beta_2|} \tag{2.1.3}$$

uniformly in $\varepsilon \in (0,1]$, hence the set $\mathcal{W} := \{\chi_\varepsilon w : \varepsilon \in (0,1]\}$ satisfies the assumptions of Proposition A.3.2. It follows that $(z - H^{(\mu,\varepsilon)})^{-1} \in \mathrm{Op}(S(\langle \xi, \zeta\rangle^{-m}))$ with all symbolic bounds uniform in $\varepsilon \in (0,1]$ and blowing up algebraically as $\Im z \to 0$. Recall that $H^{(\mu)} \in \mathrm{Op}(ES^m_{1,0})$ whenever $\mu > 0$ is sufficiently small, thus the same can be said of the (ε-independent) operator $(z - H^{(\mu)})^{-1}$. With $\Theta^{(\varepsilon)} := \phi(H^{(\mu,\varepsilon)}) - \phi(H^{(\mu)})$ and $W_\varepsilon := \mathrm{Op}((1-\chi_\varepsilon)w)$, the Helffer-Sjöstrand formula and Proposition A.2.1 then imply that

$$\Theta^{(\varepsilon)} = \frac{\mu}{\pi}\int_{\mathbb{C}} \bar\partial\tilde\phi(z)(z - H^{(\mu,\varepsilon)})^{-1} W_\varepsilon (z - H^{(\mu)})^{-1} d^2z \in \mathrm{Op}(\mu S(\langle \xi, \zeta\rangle^{-m})) \tag{2.1.4}$$

uniformly in $\mu > 0$ sufficiently small and $\varepsilon \in (0,1]$. Since ϕ is arbitrary, we also have that $\Theta_0^{(\varepsilon)} := \phi_0(H^{(\mu,\varepsilon)}) - \phi_0(H^{(\mu)}) \in \mathrm{Op}(\mu S(\langle \xi, \zeta\rangle^{-m}))$ uniformly in μ and ε. Thus if $\mu > 0$ is small enough, then $(1 - \Theta_0^{(\varepsilon)})^{-1} \in \mathrm{Op}(S(1))$ uniformly in $\varepsilon \in (0,1]$. Since $\phi(H^{(\mu)}) \in$

$\mathrm{Op}(S(\langle y,\xi,\zeta\rangle^{-\infty}))$, the familiar identity

$$\Theta^{(\varepsilon)} = (\phi(H^{(\mu)})\Theta_0^{(\varepsilon)} + \Theta^{(\varepsilon)}\phi_0(H^{(\mu)}))(1-\Theta_0^{(\varepsilon)})^{-1}$$

implies that $\phi(H^{(\mu,\varepsilon)}) = \Theta^{(\varepsilon)} + \phi(H^{(\mu)}) \in \mathrm{Op}(S(\langle y,\xi,\zeta\rangle^{-\infty}))$ uniformly in $\varepsilon \in (0,1]$.

As in the proof of Theorem 2.1.7, cyclicity of the trace implies that

$$\begin{aligned}&\sigma_I(H^{(\mu,\varepsilon)},P,\varphi) - \sigma_I(H^{(\mu)},P,\varphi) = \\ &\qquad \mathrm{Tr}\, i[\Psi(H^{(\mu,\varepsilon)}),P](\varphi'(H^{(\mu,\varepsilon)}) - \varphi'(H^{(\mu)})) - \mathrm{Tr}\, i[\varphi'(H^{(\mu)}),P](\Psi(H^{(\mu,\varepsilon)}) - \Psi(H^{(\mu)})).\end{aligned}$$

Thus it suffices to show that $\mathrm{Tr}[A_\varepsilon,P]B_\varepsilon \to 0$ as $\varepsilon \downarrow 0$, for $A_\varepsilon \in \{\varphi'(H^{(\mu)}), \Psi(H^{(\mu,\varepsilon)})\}$ and $B_\varepsilon \in \{\varphi'(H^{(\mu,\varepsilon)}) - \varphi'(H^{(\mu)}), \Psi(H^{(\mu,\varepsilon)}) - \Psi(H^{(\mu)})\}$. In the paragraph above, we showed that $A_\varepsilon \in \mathrm{Op}(S(\langle y,\xi,\zeta\rangle^{-\infty}))$ uniformly in $\varepsilon \in (0,1]$. The composition calculus then implies that $[A_\varepsilon,P] \in \mathrm{Op}(S(\langle x,y,\xi,\zeta\rangle^{-\infty}))$ uniformly in $\varepsilon \in (0,1]$. Using (2.1.4) and the paragraph above it, we see that $B_\varepsilon \in \mathrm{Op}(S(1-\chi_\varepsilon(x,y,\xi,\zeta)+\varepsilon))$ uniformly in $\varepsilon \in (0,1]$. We thus have $[A_\varepsilon,P]B_\varepsilon \in \mathrm{Op}(S(\langle x,y,\xi,\zeta\rangle^{-5}(1-\chi_\varepsilon(x,y,\xi,\zeta)+\varepsilon)))$ uniformly in $\varepsilon \in (0,1]$, meaning that (see appendix A.1)

$$\begin{aligned}\|[A_\varepsilon,P]B_\varepsilon\|_1 &\le C\int_{\mathbb{R}^4} \langle x,y,\xi,\zeta\rangle^{-5}(1-\chi_\varepsilon(x,y,\xi,\zeta)+\varepsilon)\,dxdyd\xi d\zeta \\ &\le C\Big(\int_{\{|(x,y,\xi,\zeta)|\ge\varepsilon^{-1}\}} \langle x,y,\xi,\zeta\rangle^{-5} dxdyd\xi d\zeta + \varepsilon\int_{\mathbb{R}^4}\langle x,y,\xi,\zeta\rangle^{-5}dxdyd\xi d\zeta\Big) \\ &\le C\varepsilon.\end{aligned}$$

This completes the proof. □

Theorem 2.1.8 implies the following

Corollary 2.1.9. *Let $P(x) = P \in \mathfrak{S}(0,1)$ and $\varphi \in \mathfrak{S}(0,1;\tilde{E}_1,\tilde{E}_2)$. Suppose $W \in \mathrm{Op}(S^m_{1,0})$*

is symmetric such that $H^{(\mu)}$ satisfies (H0) for all $\mu \in [0,1]$. Then

$$\sigma_I(H^{(1)}, P, \varphi) = \sigma_I(H, P, \varphi).$$

Proof. For any $\mu \in [0,1]$, Theorem 2.1.8 implies that $\sigma_I(H^{(\mu')}, P, \varphi)$ is constant over μ' in some small neighborhood of μ. Thus $\sigma_I(H^{(\mu)}, P, \varphi)$ is independent of $\mu \in [0,1]$, and the result is complete. $\square$

We now turn our attention to operators H satisfying (H1) in Section 1. First, we show that the latter is a stronger assumption than (H0), meaning that all the previous results obtained in this section still apply.

Proposition 2.1.10. *Suppose $H = \mathrm{Op}(\sigma)$ satisfies (H1) and $\Phi \in \mathcal{C}_c^\infty(E_1, E_2)$. Define $H_h := \mathrm{Op}_h(\sigma)$ for $h \in (0,1]$. Then $\Phi(H_h) \in \mathrm{Op}_h(S(\langle y, \xi, \zeta\rangle^{-\infty}))$.*

Proof. We observe that $H_h = \mathrm{Op}_1(\sigma(x, y, h\xi, h\zeta))$ satisfies (H1) for all $0 < h \le 1$, with $\sigma_\pm(h\xi, h\zeta)$ replacing $\sigma_\pm(\xi, \zeta)$. This means H_h is self-adjoint with domain $\mathcal{H}^m$ that is dense in $\mathcal{H}$, and $(i + H_h)^{-1} \in \mathrm{Op}_h(S(\langle \xi, \zeta\rangle^{-m}))$ as recalled in Proposition A.3.1 below. Writing $\Phi(H_h) = (i + H_h)^{-N}\Phi_N(H_h)$ for Φ_N still compactly supported, we obtain that $\Phi(H_h) \in \mathrm{Op}_h(S(\langle \xi, \zeta\rangle^{-\infty}))$.

We now prove decay in y. Since $\sigma_\pm$ are independent of (x, y) and have a spectral gap in (E_1, E_2), it follows that $H_{\pm,h} := \mathrm{Op}_h(\sigma_\pm)$ also have a spectral gap in (E_1, E_2). Hence $\Phi(H_{\pm,h}) = 0$, meaning that

$$\Phi(H_h) = \phi(y)(\Phi(H_h) - \Phi(H_{+,h})) + (1 - \phi(y))(\Phi(H_h) - \Phi(H_{-,h})),$$

where we assume $\phi \in \mathfrak{S}(0,1)$. By the Helffer-Sjöstrand Formula, we see that

$$\Phi(H_h) - \Phi(H_{+,h}) = -\frac{1}{\pi}\int_Z \bar{\partial}\tilde{\Phi}(z)(z - H_h)^{-1}(H_h - H_{+,h})(z - H_{+,h})^{-1} d^2 z,$$

with $H_h - H_{+,h} = \mathrm{Op}_h(\sigma - \sigma_+)$ and $\sigma - \sigma_+$ vanishing for $y > 0$ sufficiently large. By Propositions A.2.1 and A.3.1 (and the rapid decay of $\bar{\partial}\tilde{\Phi}$ near the real axis), it follows that $\Phi(H_h) - \Phi(H_{+,h}) \in \mathrm{Op}_h(S(\langle y_+\rangle^{-\infty}))$. Since $\phi(y) = \phi \in \mathrm{Op}_h(S(\langle y_-\rangle^{-\infty}))$, the composition calculus implies that $\phi(y)(\Phi(H_h) - \Phi(H_{+,h})) \in \mathrm{Op}_h(\langle y\rangle^{-\infty})$. A parallel argument proves that $(1-\phi(y))(\Phi(H_h) - \Phi(H_{-,h})) \in \mathrm{Op}_h(\langle y\rangle^{-\infty})$, hence $\Phi(H_h) \in \mathrm{Op}_h(\langle y\rangle^{-\infty})$. The result then follows from interpolation. $\square$

We now show that under (H1), the interface conductivity is stable with respect to semiclassical rescaling.

Theorem 2.1.11. *Suppose $H = \mathrm{Op}(\sigma)$ satisfies (H1), and define $H_h := \mathrm{Op}_h(\sigma)$. Let $P(x) = P \in \mathfrak{S}(0,1)$ and $\varphi \in \mathfrak{S}(0,1;E_1,E_2)$. Then $\sigma_I(H_h, P, \varphi) = \sigma_I(H, P, \varphi)$ for all $h \in (0,1]$.*

Proof. Fix $h \in (0,1]$. Since $H_h = \mathrm{Op}(\sigma_h)$ with $\sigma_h(x,y,\xi,\zeta) = \sigma(x,y,h\xi,h\zeta)$, we know that H_h satisfies (H1). Observe also that for any $h' \in (0,1]$, we have $H_h - H_{h'} \in \mathrm{Op}(S^m_{1,0})$. For $h' \in (0,1]$ and $\mu \in [0,1]$, define $\sigma^{(\mu)}_{h,h'} := \sigma_h + \mu(\sigma_{h'} - \sigma_h)$. By continuity and ellipticity of σ, we know that whenever $|h'-h|$ is sufficiently small, $\sigma^{(\mu)}_{h,h'} \in ES^m_{1,0}$ for all $\mu \in [0,1]$. Moreover, (H1) implies that $\sigma^{(\mu)}_{h,h'}(x,y,\xi,\zeta) = \sigma^{(\mu)}_{h,h',\pm}(\xi,\zeta)$ whenever $\pm y$ is sufficiently large, where

$$\sigma^{(\mu)}_{h,h',\pm}(\xi,\zeta) := \sigma_\pm(h\xi,h\zeta) + \mu(\sigma_\pm(h'\xi h'\zeta) - \sigma_\pm(h\xi,h\zeta)).$$

Since $\sigma_\pm$ have a spectral gap in (E_1,E_2), it follows (also from $\sigma^{(\mu)}_{h,h'} \in ES^m_{1,0}$ and continuity) that whenever $|h'-h|$ is sufficiently small, $\sigma^{(\mu)}_{h,h',\pm}$ has a spectral gap in $(E_1+\Delta, E_2-\Delta)$ for all $\mu \in [0,1]$, where $\Delta := (E_2-E_1)/4$. Thus we have shown that whenever $|h'-h|$ is sufficiently small and $\mu \in [0,1]$, the operator $H^{(\mu)}_{h,h'} := \mathrm{Op}(\sigma^{(\mu)}_{h,h'})$ satisfies (H1) with (E_1,E_2) replaced by $(E_1+\Delta, E_2-\Delta)$. By Theorem 2.1.8, we conclude that whenever $|h'-h|$ is sufficiently small, $\sigma_I(H^{(\mu)}_{h,h'}, P, \varphi_1)$ is independent of $\mu \in [0,1]$, provided $\varphi_1 \in \mathfrak{S}(0,1;E_1+\Delta,E_2-\Delta)$. In particular, this means $\sigma_I(H_{h'}, P, \varphi_1) = \sigma_I(H_h, P, \varphi_1)$ if $|h'-h|$ is sufficiently small. But since $H_{h'}$ satisfies (H1), we know by Proposition 2.1.3 that $\sigma_I(H_{h'}, P, \varphi) = \sigma_I(H_h, P, \varphi)$. We have thus shown that $\sigma_I(H_{h'}, P, \varphi)$ is constant over h' in some small neighborhood of h. Since $h \in (0, 1]$ was arbitrary, the result is complete. $\square$

Finally, we show that the interface conductivity is immune to oscillations in the x-variable.

Theorem 2.1.12. *Suppose $H = \mathrm{Op}(\sigma)$ satisfies (H1), $P(x) = P \in \mathfrak{S}(0, 1)$ and $\varphi \in \mathfrak{S}(0, 1; E_1, E_2)$. Fix $x_0 \in \mathbb{R}$ and define $\sigma_{x_0}(x, y, \xi, \zeta) := \sigma(x_0, y, \xi, \zeta)$ and $H_{x_0} := \mathrm{Op}(\sigma_{x_0})$. Then $\sigma_I(H_{x_0}, P, \varphi) = \sigma_I(H, P, \varphi)$.*

Proof. Let $\chi \in \mathcal{C}_c^\infty(-2, 2)$ such that $\chi(x) = 1$ whenever $x \in [-1, 1]$. Define $\chi_\varepsilon(x) := \chi(\varepsilon x)$. For $\varepsilon \in (0, 1]$, define $\sigma^{(\varepsilon)}(x, y, \xi, \zeta) := \sigma(x - (x - x_0)\chi_\varepsilon(x - x_0), y, \xi, \zeta)$, so that $\sigma^{(\varepsilon)} = \sigma_{x_0}$ whenever $|x - x_0| \le \varepsilon^{-1}$ and $\sigma^{(\varepsilon)} = \sigma$ whenever $|x - x_0| \ge 2\varepsilon^{-1}$. Since $H^{(\varepsilon)} := \mathrm{Op}(\sigma^{(\varepsilon)})$ satisfies (H1) and $\sigma^{(\varepsilon)} - \sigma$ vanishes whenever $\langle x, y\rangle$ is sufficiently large, Theorem 2.1.5 implies that $\sigma_I(H^{(\varepsilon)}, P, \varphi) = \sigma_I(H, P, \varphi)$ for all $\varepsilon \in (0, 1]$.

It remains to show that $\sigma_I(H^{(\varepsilon)}, P, \varphi) - \sigma_I(H_{x_0}, P, \varphi) \to 0$ as $\varepsilon \downarrow 0$. To do this, we will emulate the argument used to prove Theorem 2.1.8. In particular, it suffices to show that $\mathrm{Tr}[A_\varepsilon, P]B_\varepsilon \to 0$ as $\varepsilon \downarrow 0$, for $A_\varepsilon \in \{\phi(H_{x_0}), \phi(H^{(\varepsilon)})\}$, $B_\varepsilon = \phi(H^{(\varepsilon)}) - \phi(H_{x_0})$ and $\phi \in \mathcal{C}_c^\infty(E_1, E_2)$. As before, Proposition A.3.2 and the composition calculus imply that $[A_\varepsilon, P] \in \mathrm{Op}(S(\langle x, y, \xi, \zeta\rangle^{-\infty}))$ uniformly in $\varepsilon \in (0, 1]$. By the Helffer-Sjöstrand formula,

$$B_\varepsilon = \frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\phi}(z)(z - H^{(\varepsilon)})^{-1}(H_{x_0} - H^{(\varepsilon)})(z - H_{x_0})^{-1} d^2 z.$$

Since $\sigma_{x_0} - \sigma^{(\varepsilon)}$ vanishes whenever $|x - x_0| \le \varepsilon^{-1}$, it follows that $\sigma_{x_0} - \sigma^{(\varepsilon)} \in S((1 - \chi_\varepsilon(x - x_0) + \varepsilon)\langle \xi, \zeta\rangle^m)$ uniformly in $\varepsilon \in (0, 1]$. By Propositions A.2.1 and A.3.2 (and the rapid decay of $\bar{\partial}\tilde{\phi}$ near the real axis), we conclude that $B_\varepsilon \in \mathrm{Op}(S(1 - \chi_\varepsilon(x - x_0) + \varepsilon))$ uniformly in $\varepsilon \in (0,1]$. Therefore,

$$\begin{aligned}\|[A_\varepsilon, P]B_\varepsilon\|_1 &\le C\int_{\mathbb{R}^4}\langle x\rangle^{-2}\langle y,\xi,\zeta\rangle^{-4}(1-\chi_\varepsilon(x-x_0)+\varepsilon)dxdyd\xi d\zeta\\ &\le C\int_{\mathbb{R}}\langle x\rangle^{-2}(1-\chi_\varepsilon(x-x_0)+\varepsilon)dx\\ &\le C\Big(\int_{\{|x-x_0|\ge\varepsilon^{-1}\}}\langle x\rangle^{-2}dx+\varepsilon\int_{\mathbb{R}}\langle x\rangle^{-2}dx\Big)\le C\varepsilon,\end{aligned}$$

and the proof is complete. □

2.2 Bulk-interface correspondence

In this section, we derive an integral representation of the interface conductivity σ_I in (1.0.1) that takes the form of a Fedosov-Hörmander formula (2.2.7) as in [10, 11]. We then simplify the evaluation of this integral under additional assumptions on the Hamiltonian.

The formula (2.2.7) may then be interpreted as in [10] as bulk-difference invariant; see Corollary 2.2.2. That the interface conductivity is given as bulk-difference invariant (which are defined in a more general setting than a difference of bulk-invariants) is usually referred to as a bulk-interface (or bulk-boundary) correspondence; see [7, 10, 37, 40, 42, 49, 68]. Establishing such a correspondence is one of the major objectives of mathematical analyses of topological insulators as it relates the quantized asymmetric transport, a physical observation, to the topological properties of two bulk insulators.

2.2.1 Bulk-Interface correspondence and semiclassical calculus

The aim of this section is to write the conductivity as an integral involving only the symbol σ of the Hamiltonian. As demonstrated by sections 2.2.2 and 2.3 below, this integral can be used to easily evaluate σ_I in many cases of interest. Unless one can obtain a full spectral decomposition of the Hamiltonian as in [10], the integral and its simplifications represent the most accessible formulas for the conductivity.

The main result of this section is Theorem 2.2.1 below. The formula (2.2.1) simplifies nicely in various cases of interest (see section 2.2.2), and also implies a bulk-interface correspondence (Corollary 2.2.2) and Fedosov-Hörmander formula (Corollary 2.2.3).

Theorem 2.2.1. *Suppose $H = \mathrm{Op}(\tilde{\sigma})$ satisfies (H1), $P(x) = P \in \mathfrak{S}(0,1)$ and $\varphi \in \mathfrak{S}(0,1;E_1,E_2)$. Let $\alpha \in (E_1,E_2)$, and let $R \subset \mathbb{R}^3$ be bounded with a piecewise smooth boundary ∂R. Fix $x_0 \in \mathbb{R}$, and define $\sigma(y,\xi,\zeta) := \tilde{\sigma}(x_0,y,\xi,\zeta)$. Assume R contains all points (y,ξ,ζ) where $\sigma(y,\xi,\zeta)$ has an eigenvalue of α. Then defining $z := \alpha + i\omega$ and $\sigma_z := z - \sigma$, we have that*

$$\sigma_I(H,P,\varphi) = \frac{i}{16\pi^3}\int_{\partial R}\int_{-\infty}^{+\infty}\Theta d\omega d\Sigma, \qquad \Theta := \operatorname{tr}\varepsilon_{ijk}\sigma_z^{-1}\partial_i\sigma_z\sigma_z^{-1}\partial_j\sigma_z\sigma_z^{-1}\nu_k \tag{2.2.1}$$

where ν is the unit vector (outwardly) normal to ∂R, $d\Sigma = d\Sigma(y,\xi,\zeta)$ is the Euclidean measure on ∂R, and ε_{ijk} is the anti-symmetric tensor with $\varepsilon_{123} = 1$ and the variables identified by $(1,2,3) = (y,\xi,\zeta)$.

The strategy for the proof is to use an asymptotic expansion in the semiclassical parameter h and apply Theorem 2.1.11 to eliminate terms that are not $O(1)$. A similar technique is used in [10, 11].

Proof. By Proposition 2.1.3, $\sigma_I(H,P,\varphi)$ is independent of $\varphi \in \mathfrak{S}(0,1;E_1,E_2)$, thus we can take $\varphi' \in \mathcal{C}_c^\infty(\alpha_0,\alpha)$ for some $\alpha_0 > E_1$. Moreover, by Theorem 2.1.12, we can without loss of generality assume that $\tilde{\sigma}(x,y,\xi,\zeta) = \sigma(y,\xi,\zeta)$ for all $(x,y,\xi,\zeta) \in \mathbb{R}^4$. Theorem 2.1.11 states that with $H_h := \mathrm{Op}_h(\tilde{\sigma})$, $\sigma_I(H_h,P,\varphi)$ is independent of $h \in (0,1]$. Thus we will expand $\sigma_I(H_h,P,\varphi)$ in powers of h and ignore terms that are not $O(1)$. We will use the shorthand $\sigma_I := \sigma_I(H_h,P,\varphi)$.

Let $\operatorname{Op}_h \nu_h := \varphi'(H_h)$. By Proposition A.3.3, we have

$$\nu_h + \frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\varphi}'(z)\tilde{q}_{z,h} d^2 z \in S^{-3/2}(\langle y, \xi, \zeta\rangle^{-\infty}), \tag{2.2.2}$$

where

$$\tilde{q}_{z,h} = \sigma_z^{-1} + \frac{ih}{2}\{\sigma_z^{-1}, \sigma_z\}_{\zeta,y}\sigma_z^{-1}, \qquad \{a,b\}_{\zeta,y} := \partial_\zeta a \partial_y b - \partial_y a \partial_\zeta b,$$

and the right-hand side of (2.2.2) is defined by (A.1.2). With $\operatorname{Op}_h(\kappa_h) := [H_h, P]$, we have that

$$\kappa_h + ihk_1 - \frac{h^2}{4}k_2 \in S^{-3}(\langle x\rangle^{-\infty}\langle \xi,\zeta\rangle^m), \qquad k_1 := \partial_\xi \sigma P'(x), \qquad k_2 := \partial_{\xi\xi}\sigma P''(x).$$

Since $\nu_h \in S(\langle y,\xi,\zeta\rangle^{-\infty})$ and $\kappa_h \in S^{-1}(\langle x\rangle^{-\infty}\langle\xi,\zeta\rangle^m)$, the composition calculus implies that

$$\kappa_h \sharp_h \nu_h - \kappa_h\nu_h + \frac{ih}{2}\{\kappa_h, \nu_h\} \in S^{-3}(\langle x, y, \xi, \zeta\rangle^{-\infty}), \tag{2.2.3}$$

where

$$\{a,b\} := \partial_\xi a \partial_x b + \partial_\zeta a \partial_y b - \partial_x a \partial_\xi b - \partial_y a \partial_\zeta b.$$

Note that S^{-3} (rather than S^{-2}) appears on the right-hand side of (2.2.3) because κ_h is $O(h)$ in $S(\langle x\rangle^{-\infty}\langle\xi,\zeta\rangle^m)$. Therefore,

$$\sigma_I = \frac{i}{(2\pi h)^2}\operatorname{tr}\int_{\mathbb{R}^4}\kappa_h\sharp_h\nu_h dR_4 = \frac{i}{(2\pi h)^2}\operatorname{tr}\int_{\mathbb{R}^4}\Big(\kappa_h\nu_h - \frac{ih}{2}\{\kappa_h,\nu_h\}\Big)dR_4 + o(1)$$

as $h \to 0$, with $dR_4 := dxdyd\xi d\zeta$. Since

$$\kappa_h \nu_h = (ihk_1 - \frac{h^2}{4}k_2)\frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\varphi}'(z)\Big(\sigma_z^{-1} + \frac{ih}{2}\{\sigma_z^{-1}, \sigma_z\}_{\zeta,y}\sigma_z^{-1}\Big)d^2z + h^{5/2}a_h$$

with $a_h \in S(\langle x, y, \xi, \zeta\rangle^{-\infty})$, and

$$\{\kappa_h, \nu_h\} = \Big\{ihk_1, \frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\varphi}'(z)\sigma_z^{-1}d^2z\Big\} + h^2 b_h, \qquad b_h \in S(\langle x, y, \xi, \zeta\rangle^{-\infty}),$$

it follows that

$$\begin{aligned}\sigma_I = \frac{i}{(2\pi h)^2}\frac{1}{\pi}\operatorname{tr}\int_{\mathbb{R}^4}\int_{\mathbb{C}} \bar{\partial}\tilde{\varphi}'(z)\Big(&ihk_1\sigma_z^{-1} - \frac{h^2}{2}k_1\{\sigma_z^{-1}, \sigma_z\}_{\zeta,y}\sigma_z^{-1} \\ &- \frac{h^2}{4}k_2\sigma_z^{-1} + \frac{h^2}{2}\{k_1, \sigma_z^{-1}\}\Big)d^2z dR_4 + o(1)\end{aligned}$$

as $h \to 0$. Since σ_I is independent of h, it follows that the $O(h^{-1})$ term above vanishes, and thus

$$\sigma_I = \frac{i}{(2\pi)^3}\operatorname{tr}\int_{\mathbb{R}^4}\int_{\mathbb{C}} \bar{\partial}\tilde{\varphi}'(z)\Big(-k_1\sigma_z^{-1}\{\sigma_z, \sigma_z^{-1}\}_{\zeta,y} - \frac{1}{2}k_2\sigma_z^{-1} + \{k_1, \sigma_z^{-1}\}\Big)d^2z dR_4. \tag{2.2.4}$$

Observe that whenever $(y, \xi, \zeta) \notin R$, $z \mapsto \sigma_z^{-1}$ is holomorphic and thus the above integral over z vanishes (this is verified via an integration by parts in $\bar{\partial}$). Since k_1 and k_2 vanish whenever $|x|$ is sufficiently large, the integration region $\mathbb{R}^4$ in (2.2.4) can be replaced by the volume $I \times R$, with $I \subset \mathbb{R}$ a bounded interval.

Recalling that $\partial_x\sigma \equiv 0$, it follows that $\{k_1, \sigma_z^{-1}\} = P'(x)\{\partial_\xi\sigma, \sigma_z^{-1}\}_{\zeta,y} - P''(x)\partial_\xi\sigma\partial_\xi\sigma_z^{-1}$ in (2.2.4). Using that $\int P' = 1$ and $\int P'' = 0$, we apply Fubini's Theorem and integrate

(2.2.4) in x to obtain

$$\sigma_I = \frac{i}{(2\pi)^3} \operatorname{tr} \int_R \int_{\mathbb{C}} \bar{\partial}\tilde{\varphi}'(z) \Big(\partial_\xi \sigma_z \sigma_z^{-1} \{\sigma_z, \sigma_z^{-1}\}_{\zeta,y} - \{\partial_\xi \sigma_z, \sigma_z^{-1}\}_{\zeta,y} \Big) d^2 z dR_3, \qquad (2.2.5)$$

with $dR_3 := dy d\xi d\zeta$. At this point, we use the identity $\{a,b\}_{\zeta,y} = \partial_\zeta(a\partial_y b) - \partial_y(a\partial_\zeta b)$ and integration by parts in (ζ, y) to write

$$\int_R \int_{\mathbb{C}} \bar{\partial}\tilde{\varphi}'(z) \{\partial_\xi \sigma_z, \sigma_z^{-1}\}_{\zeta,y} d^2 z dR_3 = \int_{\partial R} \int_{\mathbb{C}} \bar{\partial}\tilde{\varphi}'(z) \partial_\xi \sigma_z (\partial_y \sigma_z^{-1} \nu_\zeta - \partial_\zeta \sigma_z^{-1} \nu_y) d^2 z d\Sigma. \qquad (2.2.6)$$

Since $z \mapsto \sigma_z^{-1}$ is holomorphic whenever $(y,\xi,\zeta) \in \partial R$, an integration by parts in $\bar{\partial}$ reveals that the right-hand side of (2.2.6) vanishes. Thus we are left with

$$\sigma_I = \frac{i}{(2\pi)^3} \operatorname{tr} \int_R \int_{\mathbb{C}} \bar{\partial}\tilde{\varphi}'(z) \partial_\xi \sigma_z \sigma_z^{-1} \{\sigma_z, \sigma_z^{-1}\}_{\zeta,y} d^2 z dR_3.$$

Integrating by parts in $\bar{\partial}$ with $z =: \lambda + i\omega$, we see that

$$\sigma_I = \frac{1}{2(2\pi)^3} \operatorname{tr} \int_R \int_{\alpha_0}^{\alpha} \varphi'(\lambda) \partial_\xi \sigma_z \sigma_z^{-1} \{\sigma_z, \sigma_z^{-1}\}_{\zeta,y} \Big|_{\omega=0^-}^{\omega=0^+} d\lambda dR_3.$$

Since $\partial_\xi \sigma_z \sigma_z^{-1} \{\sigma_z, \sigma_z^{-1}\}_{\zeta,y} \to 0$ as $|\omega| \to \infty$, we have

$$\partial_\xi \sigma_z \sigma_z^{-1} \{\sigma_z, \sigma_z^{-1}\}_{\zeta,y} \Big|_{\omega=0^-}^{\omega=0^+} = - \int_{-\infty}^{+\infty} \partial_\omega (\partial_\xi \sigma_z \sigma_z^{-1} \{\sigma_z, \sigma_z^{-1}\}_{\zeta,y}) d\omega.$$

Cyclicity of the trace and the fact that $\partial_\omega \sigma_z = i$ imply that

$$\operatorname{tr} \partial_\omega (\partial_\xi \sigma_z \sigma_z^{-1} \{\sigma_z, \sigma_z^{-1}\}_{\zeta,y}) = -i \operatorname{tr} \varepsilon_{ijk} \partial_k (\sigma_z^{-1} \partial_i \sigma_z \sigma_z^{-1} \partial_j \sigma_z \sigma_z^{-1}),$$

where ε_{ijk} is the anti-symmetric tensor with $\varepsilon_{123} = 1$, and the variables are identified by

$(1,2,3)=(y,\xi,\zeta)$. Pulling ∂_k out of the integral over ω and integrating by parts, we get

$$\operatorname{tr}\int_R \partial_\xi\sigma_z\sigma_z^{-1}\{\sigma_z,\sigma_z^{-1}\}_{\zeta,y}\Big|_{\omega=0^-}^{\omega=0^+} dR_3 = i\int_{\partial R}\int_{-\infty}^{+\infty}\Theta d\omega d\Sigma,$$

where we recall the definition of Θ in (2.2.1). Thus we have shown that

$$\sigma_I = \frac{i}{16\pi^3}\int_{[\alpha_0,\alpha]}\varphi'(\lambda)\int_{\partial R}\int_{-\infty}^{+\infty}\Theta d\omega d\Sigma d\lambda.$$

Integrating by parts in λ, we obtain

$$\sigma_I = \frac{i}{16\pi^3}\int_{\partial R}\int_{-\infty}^{+\infty}\Theta d\omega d\Sigma,$$

with now $z=\alpha+i\omega$ in the above integrand. The fact that only the boundary term survives follows from analyticity of Θ in z over the region of integration (so that $\partial_\lambda\Theta=-i\partial_\omega\Theta$). This completes the proof. $\square$

Corollary 2.2.2. *Suppose $H=\operatorname{Op}(\sigma)$ satisfies (H1), $P(x)=P\in\mathfrak{S}(0,1)$ and $\varphi\in\mathfrak{S}(0,1;E_1,E_2)$. Let $\alpha\in(E_1,E_2)$ and define $\tau_{\pm,z}:=z-\sigma_\pm$ with $z=\alpha+i\omega$. Then*

$$2\pi\sigma_I(H,P,\varphi)=\frac{i}{8\pi^2}(I_+-I_-),\qquad I_\pm=\int_{\mathbb{R}^3}\operatorname{tr}[\tau_{\pm,z}^{-1}\partial_\xi\tau_{\pm,z},\tau_{\pm,z}^{-1}\partial_\zeta\tau_{\pm,z}]\tau_{\pm,z}^{-1}d\omega d\xi d\zeta.$$

Proof. Fix $y_0>0$ sufficiently large, and define $R_M:=(-y_0,y_0)\times(-M,M)^2$ for all $M>0$. Observe that $|\Theta|\le C\langle\omega\rangle^{-3}$ and $|\Theta|\le C\langle\xi,\zeta\rangle^{-m-2}$ uniformly in $(y,\xi,\zeta)\in\partial R_M$ and $M>0$ sufficiently large, hence $|\Theta|\le C\langle\omega\rangle^{-3/2}\langle\xi,\zeta\rangle^{-\frac{m+2}{2}}$ by interpolation. It follows that $\int_{-\infty}^{+\infty}|\Theta|d\omega\le C\langle\xi,\zeta\rangle^{-\frac{m+2}{2}}$. Therefore, taking $R:=R_M$ in Theorem 2.2.1 and sending $M\to\infty$, we see that the contributions to σ_I in (2.2.1) from the sides of ∂R_M with normal vector in the ξ and ζ directions vanish. Indeed, the area of these surfaces is proportional to M, with the maximum of the integrand bounded by $CM^{-1-m/2}$. Thus we are left with integrals over the sides corresponding to $y=\pm y_0$, over which $\sigma(y,\xi,\zeta)=\sigma_\pm(\xi,\zeta)$. As a consequence, $\sigma_I = \frac{i}{16\pi^3}(I_+ - I_-)$, and the proof is complete. $\square$

Corollary 2.2.3. *Suppose $H = \mathrm{Op}(\tilde{\sigma})$ satisfies (H1), $P(x) = P \in \mathfrak{S}(0,1)$ and $\varphi \in \mathfrak{S}(0,1;E_1,E_2)$. Let $\alpha \in (E_1,E_2)$, and let $S \subset \mathbb{R}^4$ be bounded with a piecewise smooth boundary ∂S. Fix $x_0 \in \mathbb{R}$ and define $\sigma(y,\xi,\zeta) := \tilde{\sigma}(x_0,y,\xi,\zeta)$. Assume S contains all points $(0,y,\xi,\zeta)$ where $\sigma(y,\xi,\zeta)$ has an eigenvalue of α. Then for $z := \alpha + i\omega$ and $\sigma_z := z - \sigma$, we have that*

$$2\pi\sigma_I(H,P,\varphi) = \frac{1}{24\pi^2}\int_{\partial S} u \cdot \nu d\Sigma_3, \qquad u_l := \operatorname{tr} \epsilon_{ijkl}\partial_i\sigma_z\sigma_z^{-1}\partial_j\sigma_z\sigma_z^{-1}\partial_k\sigma_z\sigma_z^{-1}, \quad (2.2.7)$$

where ν is the outward unit normal to ∂S, $d\Sigma_3 = d\Sigma_3(\omega,y,\xi,\zeta)$ is the Euclidean measure on ∂S, and ϵ_{ijkl} the anti-symmetric tensor with $\epsilon_{1234} = 1$ and the variables identified by $(1,2,3,4) = (\omega,y,\xi,\zeta)$.

Observe that we can write the above integral in a more geometric form:

$$\int_{\partial S} u \cdot \nu d\Sigma_3 = \int_{\partial S} (\sigma_z^{-1} d\sigma_z)^3.$$

Proof. By Theorem 2.2.1,

$$\sigma_I = \frac{i}{16\pi^3}\lim_{M\to\infty}\int_{\partial R}\int_{-M}^{M} \Theta d\omega d\Sigma. \quad (2.2.8)$$

Since $|\Theta| \le C\langle\omega\rangle^{-3}$, it follows that if $z = \alpha \pm iM$ and $i,j,k \in \{\omega,y,\xi,\zeta\}$, then

$$\int_R |\operatorname{tr}\partial_i\sigma_z\sigma_z^{-1}\partial_j\sigma_z\sigma_z^{-1}\partial_k\sigma_z\sigma_z^{-1}| dR_3 \longrightarrow 0 \quad (2.2.9)$$

as $M \to \infty$. Since $\partial_\omega\sigma = i$, we know that

$$\Theta = -i\operatorname{tr}\varepsilon_{ijk}\partial_\omega\sigma\sigma_z^{-1}\partial_i\sigma_z\sigma_z^{-1}\partial_j\sigma_z\sigma_z^{-1}\nu_k. \quad (2.2.10)$$

It then follows from cyclicity of the trace that

$$\sigma_I = \frac{1}{48\pi^3} \lim_{M\to\infty} \int_{\partial S_M} u \cdot \nu d\Sigma_3, \tag{2.2.11}$$

where $S_M := [-M, M] \times R$. Indeed, the integral over $[-M, M] \times \partial R \subset \partial S_M$ is precisely the integral on the right-hand side of (2.2.8), while the integral over the rest of ∂S_M vanishes in the $M \to \infty$ limit by (2.2.9). The factor of 3 adjustment in (2.2.11) compared to (2.2.8) is justified by the rank-four tensor ϵ_{ijkl}, which causes each term on the right-hand side of (2.2.10) to appear three times in (2.2.11).

By assumption, all singularities of σ_z^{-1} lie in $S_M \cap S$ when M is sufficiently large. Hence σ_z^{-1} is well-defined in $S_M \Delta S := (S_M \cup S) \setminus (S \cap S_M)$. It follows that for $(\omega, y, \xi, \zeta) \in S_M \Delta S$, we have

$$\begin{aligned}
\nabla \cdot u &= \epsilon_{ijkl} \operatorname{tr} \partial_l (\partial_i \sigma_z \sigma_z^{-1} \partial_j \sigma_z \sigma_z^{-1} \partial_k \sigma_z \sigma_z^{-1}) \\
&= -\epsilon_{ijkl} \operatorname{tr} \Big(\partial_i \sigma_z \sigma_z^{-1} \partial_l \sigma_z \sigma_z^{-1} \partial_j \sigma_z \sigma_z^{-1} \partial_k \sigma_z \sigma_z^{-1} + \partial_i \sigma_z \sigma_z^{-1} \partial_j \sigma_z \sigma_z^{-1} \partial_l \sigma_z \sigma_z^{-1} \partial_k \sigma_z \sigma_z^{-1} \\
&\qquad + \frac{1}{2} \partial_i \sigma_z \sigma_z^{-1} \partial_j \sigma_z \sigma_z^{-1} \partial_k \sigma_z \sigma_z^{-1} \partial_l \sigma_z \sigma_z^{-1} + \frac{1}{2} \partial_l \sigma_z \sigma_z^{-1} \partial_i \sigma_z \sigma_z^{-1} \partial_j \sigma_z \sigma_z^{-1} \partial_k \sigma_z \sigma_z^{-1} \Big) \\
&= 0,
\end{aligned}$$

where we have used cyclicity of the trace to justify the second equality, and the antisymmetry of ϵ_{ijkl} for the last equality (the third term cancels half the second term, the fourth term cancels half the first term, half the second term cancels half the first term). Using the Divergence Theorem, we thus replace ∂S_M in (2.2.11) by ∂S and the proof is complete. □

2.2.2 Computing the conductivity

This section contains two simplifications of Theorem 2.2.1 that will become useful when calculating the interface conductivity for systems of interest. The first result (Proposition

2.2.4) is more general, as it requires σ to have differentiable eigenvalues and eigenvectors (up to a set of measure zero), and makes no additional assumptions besides (H1). The second (Proposition 2.2.5) provides an accessible formula for the conductivity as the degree of an appropriate map, but is restricted to certain two-dimensional models.

Throughout, we will use the shorthand $\sigma_I := \sigma_I(H, P, \varphi)$, where it is implied that $P(x) = P \in \mathfrak{S}(0,1)$ and $\varphi \in \mathfrak{S}(0,1;E_1,E_2)$. Recall Propositions 2.1.3 and 2.1.4, which state that σ_I is independent of φ and P.

Proposition 2.2.4. *Suppose $H = \mathrm{Op}(\sigma)$ satisfies (H1). Fix $x_0 \in \mathbb{R}$ and let $\lambda_\ell(y,\xi,\zeta)$ denote the eigenvalues of $\sigma(x_0,y,\xi,\zeta)$, and $\psi_\ell(y,\xi,\zeta)$ the corresponding eigenvectors. Given $E_1 < \alpha < E_2$ and R as in Theorem 2.2.1, define $n_+ := \{\ell : \lambda_\ell > \alpha \text{ on } \partial R\}$ and $n_- := \{\ell : \lambda_\ell < \alpha \text{ on } \partial R\}$. Assume that the λ_ℓ and ψ_ℓ are differentiable on ∂R, up to a set of Σ-measure zero. Then*

$$2\pi\sigma_I = \frac{i}{2\pi}\int_{\partial R}\varepsilon_{ijk}\sum_{\ell_+\in n_+,\ell_-\in n_-}\partial_i\psi^*_{\ell_+}\psi_{\ell_-}\psi^*_{\ell_-}\partial_j\psi_{\ell_+}\nu_k d\Sigma. \tag{2.2.12}$$

Proof. Recall that by the definition of ∂R, $n_+ \cup n_- = \{1,2,\dots,n\}$. Define the projectors $\Pi_\ell := \psi_\ell\psi_\ell^*$. We know that $\sigma = \sum_{\ell=1}^n \lambda_\ell \Pi_\ell$, and hence $\sigma_z^{-1} = \sum_{\ell=1}^n (z-\lambda_\ell)^{-1}\Pi_\ell$ whenever $\Im z \neq 0$. It follows from (2.2.1) and cyclicity of the trace that

$$2\pi\sigma_I = \frac{i}{8\pi^2}\int_{\partial R}\int_{\mathbb{R}}\sum_{\ell_1,\ell_2=1}^n (z-\lambda_{\ell_1})^{-2}(z-\lambda_{\ell_2})^{-1}d\omega\varepsilon_{ijk}\operatorname{tr}\Pi_{\ell_1}\partial_i\sigma\Pi_{\ell_2}\partial_j\sigma\nu_k d\Sigma. \tag{2.2.13}$$

If $\lambda_{\ell_1} \neq \lambda_{\ell_2}$, then

$$(z-\lambda_{\ell_1})^{-2}(z-\lambda_{\ell_2})^{-1} = (\lambda_{\ell_2}-\lambda_{\ell_1})^{-2}((z-\lambda_{\ell_2})^{-1}-(z-\lambda_{\ell_1})^{-1}) - (\lambda_{\ell_2}-\lambda_{\ell_1})^{-1}(z-\lambda_{\ell_1})^{-2}.$$

Thus the integral over ω vanishes if $\lambda_{\ell_1}-\alpha$ and $\lambda_{\ell_2}-\alpha$ have the same sign, and otherwise equals $2\pi(\lambda_{\ell_2} - \lambda_{\ell_1})^{-2}$. It follows that

$$2\pi\sigma_I = \frac{i}{2\pi}\int_{\partial R}\sum_{\ell_+\in n_+,\ell_-\in n_-}(\lambda_{\ell_+} - \lambda_{\ell_-})^{-2}\varepsilon_{ijk}\operatorname{tr}\Pi_{\ell_+}\partial_i\sigma\Pi_{\ell_-}\partial_j\sigma\nu_k d\Sigma,$$

where we have added the contributions of $(\ell_1,\ell_2)\in n_+\times n_-$ and $(\ell_1,\ell_2)\in n_-\times n_+$ in (2.2.13). Finally, we observe that

$$\begin{aligned}\operatorname{tr}\Pi_{\ell_+}\partial_i\sigma\Pi_{\ell_-}\partial_j\sigma &= \operatorname{tr}(\lambda_{\ell_+}^2\Pi_{\ell_+}\partial_i\Pi_{\ell_+}\Pi_{\ell_-}\partial_j\Pi_{\ell_+} + \lambda_{\ell_+}\lambda_{\ell_-}\Pi_{\ell_+}\partial_i\Pi_{\ell_+}\Pi_{\ell_-}\partial_j\Pi_{\ell_-}\\ &\quad + \lambda_{\ell_+}\lambda_{\ell_-}\Pi_{\ell_+}\partial_i\Pi_{\ell_-}\Pi_{\ell_-}\partial_j\Pi_{\ell_+} + \lambda_{\ell_-}^2\Pi_{\ell_+}\partial_i\Pi_{\ell_-}\Pi_{\ell_-}\partial_j\Pi_{\ell_-})\\ &= -(\lambda_{\ell_+} - \lambda_{\ell_-})^2\operatorname{tr}\psi_{\ell_+}\partial_i\psi_{\ell_+}^*\psi_{\ell_-}\partial_j\psi_{\ell_-}^*\\ &= (\lambda_{\ell_+} - \lambda_{\ell_-})^2\partial_i\psi_{\ell_+}^*\psi_{\ell_-}\psi_{\ell_-}^*\partial_j\psi_{\ell_+},\end{aligned}$$

and the result is complete. $\square$

We now simplify Theorem 2.2.1 for a large class of 2-dimensional models. An analogous result for tight-binding models can be found in the literature [46]. For the current (non tight-binding) setting, one can find a similar result in [42] that expresses topological invariants in terms of the resolvent $(i\omega - H)^{-1}$. Our result is unique in that it provides a simple explicit expression for σ_I that can easily be computed without the resolvent or a spectral decomposition.

We say that a point $a\in\mathbb{R}^d$ is a *regular value* of a map $f:\mathbb{R}^d\to\mathbb{R}^d$ if the preimage $f^{-1}(a)$ is a finite collection of points $\{x_1, x_2, \ldots, x_p\}\subset\mathbb{R}^d$ such that the Jacobian $M_j^{mn} = \partial_m f_n|_{x_j}$ is nonsingular for all j. We let $\mathcal{R}(f)$ denote the set of all regular values of f. By Sard's Theorem [75], we know that $\mathbb{R}^d\setminus\mathcal{R}(f)$ has measure zero.

Proposition 2.2.5. *Let $H = \operatorname{Op}(\sigma)$ satisfy (H1), and fix $x_0\in\mathbb{R}$. Suppose there exist* *(smooth and real-valued) functions* f_1, f_2, f_3 *such that*

$$\sigma(x_0, y, \xi, \zeta) = f_1(y, \xi, \zeta)\sigma_1 + f_2(y, \xi, \zeta)\sigma_2 + f_3(y, \xi, \zeta)\sigma_3$$

for all $(y, \xi, \zeta) \in \mathbb{R}^3$*, where*

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.2.14}$$

are the Pauli matrices. In particular, this means there exists a three-dimensional ball S *such that the vector field* $f := (f_1, f_2, f_3)$ *satisfies* $|f| := \sqrt{f_1^2 + f_2^2 + f_3^2} \geq \varepsilon_0$ *in* $\mathbb{R}^3 \setminus S$*, for some* $\varepsilon_0 > 0$*. Then the set* $\mathcal{R}_{\varepsilon_0} := \mathcal{R}(f) \cap \{|a| < \varepsilon_0\}$ *is nonempty. Let* $a \in \mathcal{R}_{\varepsilon_0}$*, and define* $f^{-1}(a) =: \{(y_j, \xi_j, \zeta_j)\}_{j=1}^{p}$*. Then*

$$2\pi\sigma_I = -\sum_{j=1}^{p} \operatorname{sgn} \det M_j, \tag{2.2.15}$$

where $M_j \in \mathbb{R}^{3\times 3}$ *is the Jacobian matrix defined by* $M_j^{mn} = \partial_m f_n|_{(y_j,\xi_j,\zeta_j)}$*.*

Proof. The fact that $\mathcal{R}_{\varepsilon_0} \neq \emptyset$ is an immediate consequence of Sard's Theorem [75]. Given the structure of σ, we take $\alpha = 0$ in Theorem 2.2.1, meaning that $z = i\omega$ in (2.2.1). It follows that

$$\sigma_z^{-1} = -(\omega^2 + |f|^2)^{-1}(i\omega + \sigma),$$

from which we conclude that

$$\begin{aligned} \sigma_z^{-1}\partial_i\sigma_z\sigma_z^{-1}\partial_j\sigma_z\sigma_z^{-1} &= -(\omega^2 + |f|^2)^{-3}(i\omega + \sigma)\partial_i\sigma(i\omega + \sigma)\partial_j\sigma(i\omega + \sigma) \\ = -(\omega^2 + |f|^2)^{-3}\sigma\partial_i\sigma\sigma\partial_j\sigma\sigma &+ \omega^2(\omega^2 + |f|^2)^{-3}\left(\partial_i\sigma\partial_j\sigma\sigma + \partial_i\sigma\sigma\partial_j\sigma + \sigma\partial_i\sigma\partial_j\sigma\right) + \dots, \end{aligned}$$

where we have left out terms that are odd in ω in the last line. Carrying out the integral over ω in (2.2.1), we find that

$$2\pi\sigma_I = \frac{i}{8\pi^2}\int_{\partial R}\Big(-\frac{3\pi\epsilon_{ijk}}{8|f|^5}\operatorname{tr}\sigma\partial_i\sigma\sigma\partial_j\sigma\sigma + \frac{\pi\epsilon_{ijk}}{8|f|^3}\operatorname{tr}(\partial_i\sigma\partial_j\sigma\sigma + \partial_i\sigma\sigma\partial_j\sigma + \sigma\partial_i\sigma\partial_j\sigma)\Big)\nu_k d\Sigma.$$

Simplifying the above using cyclicity of the trace and the fact that $\sigma^2 = |f|^2$, we have

$$2\pi\sigma_I = \frac{i}{16\pi}\int_{\partial R}\frac{\epsilon_{ijk}}{|f|^3}\operatorname{tr}\sigma\partial_i\sigma\partial_j\sigma\nu_k d\Sigma.$$

Using commutation relations of the Pauli matrices, we see that

$$\operatorname{tr}\sigma\partial_i\sigma\partial_j\sigma = 4i\left(f_1(\partial_i f_2\partial_j f_3 - \partial_i f_3\partial_j f_2) + [(1,2,3)\to(2,3,1)] + [(1,2,3)\to(3,1,2)]\right),$$

which we may rewrite as $4i\epsilon_{mnp}f_m\partial_i f_n\partial_j f_p$. Letting $w\in\mathbb{R}^3$ such that $w_k = \frac{\epsilon_{ijk}}{|f|^3}\operatorname{tr}\sigma\partial_i\sigma\partial_j\sigma$, we have

$$\nabla\cdot w = \frac{4i}{|f|^3}\tilde{\epsilon}_{ijk}\epsilon_{mnp}\partial_k f_m\partial_i f_n\partial_j f_p\left(1 - \frac{3f_m^2}{f_1^2+f_2^2+f_3^2}\right)$$

away from the zeros of $|f|^2$, where the only nonzero entries of $\tilde{\epsilon}_{ijk}$ are $\tilde{\epsilon}_{123} = \tilde{\epsilon}_{231} = \tilde{\epsilon}_{312} = 1$. By symmetry, we know that $\tilde{\epsilon}_{ijk}\epsilon_{mnp}f_m^2\partial_k f_m\partial_i f_n\partial_j f_p = \tilde{\epsilon}_{ijk}\epsilon_{mnp}f_n^2\partial_k f_m\partial_i f_n\partial_j f_p = \tilde{\epsilon}_{ijk}\epsilon_{mnp}f_p^2\partial_k f_m\partial_i f_n\partial_j f_p$, meaning that

$$\nabla\cdot w = \frac{4i}{|f|^3}\tilde{\epsilon}_{ijk}\epsilon_{mnp}\partial_k f_m\partial_i f_n\partial_j f_p\left(1 - \frac{f_m^2+f_n^2+f_p^2}{f_1^2+f_2^2+f_3^2}\right) = 0.$$

Thus $2\pi\sigma_I = \frac{i}{16\pi}\int_{\partial R} w\cdot\hat{\nu}d\Sigma$, where $\hat{\nu}$ is the unit vector normal to the surface ∂R and w has zero divergence everywhere except for a finite number of points in $\mathbb{R}^3$. Hence we can deform ∂R in any way so long as it encloses the same zeros of $|f|^3$. It follows that

$$2\pi\sigma_I = \frac{i}{16\pi}\int_{\partial S} w\cdot\hat{\nu}d\Sigma; \quad w\cdot\hat{\nu} = \frac{-4i}{|f|^3\sqrt{\xi^2+\zeta^2+y^2}}\det\begin{bmatrix} 0 & f_1 & f_2 & f_3 \\ \xi & \partial_\xi f_1 & \partial_\xi f_2 & \partial_\xi f_3 \\ \zeta & \partial_\zeta f_1 & \partial_\zeta f_2 & \partial_\zeta f_3 \\ y & \partial_y f_1 & \partial_y f_2 & \partial_y f_3 \end{bmatrix}.$$

Using the geometric interpretation of the determinant, we have

$$2\pi\sigma_I = -\frac{1}{4\pi}\int_{\partial S}\frac{1}{|f|^3}\det\begin{bmatrix} f_1 & f_2 & f_3 \\ \partial_u f_1 & \partial_u f_2 & \partial_u f_3 \\ \partial_v f_1 & \partial_v f_2 & \partial_v f_3 \end{bmatrix} du\wedge dv,$$

where $u = -\hat{\xi}\sin\phi + \hat{\zeta}\cos\phi$ and $v = -\hat{\xi}\cos\theta\cos\phi - \hat{\zeta}\cos\theta\sin\phi + \hat{y}\sin\theta$, with θ and ϕ the polar and azimuthal angles that parametrize ∂S. We conclude from [38, Corollary 14.2.1] and continuity of the degree of a map that $2\pi\sigma_I = -\deg g$, where $g : \partial S \to \mathbb{S}^2$ is the *Gauss map* defined by

$$(y,\xi,\zeta) \mapsto \frac{f(y,\xi,\zeta)-a}{|f(y,\xi,\zeta)-a|}.$$

The fact that $\deg g = \sum_{j=1}^{p}\operatorname{sgn}\det M_j$ is a direct consequence of [38, Theorems 14.4.3 and 14.4.4]. $\square$

2.3 Applications

We now apply the preceding results to standard Hamiltonians that appear in the analysis of topological insulators and superconductors, and in particular the 2×2 Dirac system

[7, 8, 10, 11, 68, 87]

$$H = D_x\sigma_1 + D_y\sigma_2 + m(y)\sigma_3, \tag{2.3.1}$$

and models for p-wave and d-wave superconductors following [86],

$$H = \left(\frac{1}{2m}(D_x^2 + D_y^2) - \mu\right)\sigma_1 + \frac{1}{2}(c(y)D_y + D_y c(y))\sigma_2 + c_0 D_x\sigma_3 \tag{2.3.2}$$

$$H = \left(\frac{1}{2m}(D_x^2 + D_y^2) - \mu\right)\sigma_1 + c_0(D_y^2 - D_x^2)\sigma_2 + \frac{1}{2}D_x(c(y)D_y + D_y c(y))\sigma_3. \tag{2.3.3}$$

Here, c_0, m, and μ are fixed positive constants, the σ_i are the Pauli matrices (2.2.14), and we have defined $D_\alpha := -i\partial_\alpha$. We assume that $m(y)$ and $c(y)$ are smooth domain walls with

$$m(y) = \begin{cases} m_-, & y \le -y_0 \\ m_+, & y \ge y_0 \end{cases} \qquad \text{and} \qquad c(y) = \begin{cases} c_-, & y \le -y_0 \\ c_+, & y \ge y_0 \end{cases}$$

for some $y_0 > 0$, where the constants $m_\pm$ and $c_\pm$ are all nonzero. Without loss of generality, assume $m'(y) \neq 0$ for all $y \in m^{-1}(0)$, and $c'(y) \neq 0$ for all $y \in c^{-1}(0)$.

Throughout this section, let $\sigma_{\min}$ denote the smallest-magnitude eigenvalue of σ. We continue to use the shorthand $\sigma_I := \sigma_I(H, P, \varphi)$, where $P(x) = P \in \mathfrak{S}(0,1)$ and $\varphi \in \mathfrak{S}(0,1; E_1, E_2)$ is implied.

2×2 **Dirac system** (2.3.1)**.** We have $H = \mathrm{Op}(\sigma)$, with $\sigma = \xi\sigma_1 + \zeta\sigma_2 + m(y)\sigma_3$. Thus it is clear that $\sigma \in S^1_{1,0}$ with $\sigma^2 = \xi^2 + \zeta^2 + m^2(y) \ge \xi^2 + \zeta^2$. Using that $\langle \xi, \zeta\rangle - |(\xi,\zeta)| \le 1$, it follows that $|\sigma_{\min}| \ge \langle \xi, \zeta \rangle - 1$. Now, take $\sigma_\pm := \xi\sigma_1 + \zeta\sigma_2 \pm m_\pm\sigma_3$, with $E_2 := \min\{|m_+|, |m_-|\}$ and $E_1 := -E_2$. Since $\sigma_\pm^2 = \xi^2 + \zeta^2 + m_\pm^2 \ge m_\pm^2$, (H1) is satisfied.

We now apply Proposition 2.2.5 with $f = (\xi, \zeta, m(y))$, so that $f^{-1}(0) = \{(y, 0, 0) : m(y) = 0\}$. Given a point $y \in m^{-1}(0)$, the determinant of the Jacobian of f evaluated at $(y, 0, 0)$ is $m'(y)$. Thus it follows that $2\pi\sigma_I = \frac{1}{2}(\mathrm{sgn}(m_-) - \mathrm{sgn}(m_+))$, as in e.g., [7, 10].

p-wave superconductor model (2.3.2)**.** We have $H = \mathrm{Op}(\sigma)$, with

$$\sigma = \Big(\frac{1}{2m}(\xi^2+\zeta^2)-\mu\Big)\sigma_1 + c(y)\zeta\sigma_2 + c_0\xi\sigma_3.$$

It follows that $\sigma \in S^2_{1,0}$ with, moreover, $\sigma^2 = \Big(\frac{1}{2m}(\xi^2+\zeta^2)-\mu\Big)^2 + c^2(y)\zeta^2 + c_0^2\xi^2 \geq \Big(\frac{1}{2m}(\xi^2+\zeta^2)-\mu\Big)^2$, which implies

$$|\sigma_{\min}| \geq \Big|\frac{1}{2m}(\xi^2+\zeta^2)-\mu\Big| = \Big|\frac{1}{2m}(\langle\xi,\zeta\rangle^2-1)-\mu\Big|.$$

Thus there exists $C_1 > 0$ and a compact set $K \subset \mathbb{R}^2$ such that $|\sigma_{\min}| \geq C_1\langle\xi,\zeta\rangle^2$ for all $(\xi,\zeta) \in \mathbb{R}^2 \setminus K$. Moreover, there exists $C_2 > 0$ such that $\langle\xi,\zeta\rangle^2 \leq C_2$ and hence $1+|\sigma_{\min}| \geq 1 \geq \frac{1}{C_2}\langle\xi,\zeta\rangle^2$ for all $(\xi,\zeta) \in K$. It follows that for $c := \min\{C_1, \frac{1}{C_2}\}$, we have $1+|\sigma_{\min}| \geq c\langle\xi,\zeta\rangle^2$, for $(\xi,\zeta) \in \mathbb{R}^2$. Now, take $\sigma_\pm := (\frac{1}{2m}(\xi^2+\zeta^2)-\mu)\sigma_1 + c_\pm\zeta\sigma_2 + c_0\xi\sigma_3$, so that $\sigma_\pm^2 = (\frac{1}{2m}(\xi^2+\zeta^2)-\mu)^2 + c_\pm^2\zeta^2 + c_0^2\xi^2$. Minimizing the above with respect to (ξ,ζ) is equivalent to minimizing

$$f_\pm(a,b) := \Big(\frac{1}{2m}(a+b)-\mu\Big)^2 + c_\pm^2 b + c_0^2 a$$

with respect to $(a,b) \geq 0$. We see that

$$\partial_a f_\pm = \frac{1}{m}\Big(\frac{1}{2m}(a+b)-\mu\Big) + c_0^2, \qquad \partial_b f_\pm = \frac{1}{m}\Big(\frac{1}{2m}(a+b)-\mu\Big) + c_\pm^2,$$
$$\partial^2_{aa} f_\pm = \partial^2_{ab} f_\pm = \partial^2_{bb} f_\pm = \frac{1}{2m^2},$$

hence $f_\pm$ is convex. Since $\partial_a f_\pm - \partial_b f_\pm = c_0^2 - c_\pm^2$, we know that the minimum value of $f_\pm$ is attained when either $a = 0$ or $b = 0$. We have $f_\pm(0,b) = \Big(\frac{1}{2m}b-\mu\Big)^2 + c_\pm^2 b$, which is a convex function that is minimized when $\frac{1}{m}\Big(\frac{1}{2m}b-\mu\Big) + c_\pm^2 = 0$, or equivalently $b = 2m\mu - 2m^2c_\pm^2 =: b^*$. Similarly, $f_\pm(a,0)$ is a convex function that is minimized when

$a = 2m\mu - 2m^2c_0^2 =: a^*$.

Case 1: Suppose $a^*, b^* < 0$. Then the solution for our minimization problem is $a = b = 0$, which yields a value of $f_\pm(0,0) = \frac{1}{4m^2}\mu^2$.

Case 2: Suppose $a^* < 0 < b^*$. Then the minimum value of $f_\pm$ over the allowed domain is

$$f_\pm(0,b^*) = m^2c_\pm^4 + (2m\mu - 2m^2c_\pm^2)c_\pm^2 = 2m\mu c_\pm^2 - m^2c_\pm^4 = mc_\pm^2(2\mu - mc_\pm^2),$$

which is bounded below by $m^2c_\pm^4$.

Case 3: Suppose $b^* < 0 < a^*$. Then the minimum value of $f_\pm$ over the allowed domain is

$$f_\pm(a^*,0) = m^2c_0^4 + c_0^2(2m\mu - 2m^2c_0^2) = mc_0^2(2\mu - mc_0^2),$$

which is bounded below by $m^2c_0^4$.

Case 4: Suppose $a^*, b^* > 0$. Then the minimum value of $f_\pm$ over the allowed domain is

$$\min\{f_\pm(a^*,0), f_\pm(0,b^*)\} = mc_1^2(2\mu - mc_1^2), \qquad c_1 := \min\{c_0, c_\pm\}.$$

In each case, we have proven the existence of $E_\pm > 0$ such that $\sigma_\pm^2 \geq E_\pm^2$. Define $E_0 := \min\{E_+, E_-\}$, and take $(E_1, E_2) := (-E_0, E_0)$. Thus we have verified (H1).

We now apply Proposition 2.2.5 with $f_1 = \frac{1}{2m}(\xi^2+\zeta^2)-\mu$, $f_2 = \zeta c(y)$, and $f_3 = c_0\xi$. The zeros of $f_1^2 + f_2^2 + f_3^2$ are $(y,\xi,\zeta) = (y_1, 0, \pm\sqrt{2m\mu})$, for all $y_1 \in c^{-1}(0)$. A straightforward calculation reveals that $\operatorname{sgn}\det \partial_m f_n|_{(y_1,0,\pm\sqrt{2m\mu})} = \operatorname{sgn} c'(y_1)$, hence $2\pi\sigma_I = \operatorname{sgn}(c_-) - \operatorname{sgn}(c_+)$.

d**-wave superconductor model** (2.3.3)**.** Here, the symbol of H is

$$\sigma = \Big(\frac{1}{2m}(\xi^2+\zeta^2)-\mu\Big)\sigma_1 + c_0(\zeta^2-\xi^2)\sigma_2 + \xi\zeta c(y)\sigma_3.$$

We see that $\sigma \in S^2_{1,0}$, and $\sigma^2 = (\frac{1}{2m}(\xi^2+\zeta^2)-\mu)^2 + c_0^2(\zeta^2-\xi^2)^2 + \xi^2\zeta^2c^2(y) \geq (\frac{1}{2m}(\xi^2+\zeta^2)-\mu)^2$, hence σ is elliptic. As with the p-wave superconductor, we set $\sigma_\pm$ equal to σ with $c(y)$ replaced by $c_\pm$.

We now apply Proposition 2.2.5, with $f_1 = \frac{1}{2m}(\xi^2+\zeta^2)-\mu$, $f_2 = c_0(\zeta^2-\xi^2)$, and $f_3 = \xi\zeta c(y)$. The zeros of $f_1^2+f_2^2+f_3^2$ are $(y,\xi,\zeta) = (y_1, \varepsilon_1\sqrt{m\mu}, \varepsilon_2\sqrt{m\mu})$, for all $y_1 \in c^{-1}(0)$ and $\varepsilon_1, \varepsilon_2 \in \{-1,1\}$. (That is, there are four zeros for every $y_1 \in c^{-1}(0)$.) One can then easily verify that $\operatorname{sgn}\det \partial_m f_n|_{(y_1,\varepsilon_1\sqrt{m\mu},\varepsilon_2\sqrt{m\mu})} = \operatorname{sgn} c'(y_1)$. Thus we conclude that $2\pi\sigma_I = 2(\operatorname{sgn}(c_-)-\operatorname{sgn}(c_+))$.

Regularized model of equatorial waves. The two-dimensional water wave model is given by a Hamiltonian $H_0 = \mathrm{Op}(\sigma_0)$ with

$$\sigma_0(x,y,\xi,\zeta) = \begin{pmatrix} 0 & \xi & \zeta \\ \xi & 0 & -if(y) \\ \zeta & if(y) & 0 \end{pmatrix} \tag{2.3.4}$$

where $f(y)$ is a Coriolis force that is positive when $y > 0$ (northern hemisphere of (necessarily) flat Earth) and negative when $y < 0$; see [10, 33, 79] for background on this water wave problem and in particular the observation that the bulk-interface correspondence fails for certain profiles $f(y)$ [10].

We thus consider here a regularized version given by Hamiltonian $H_\mu = \mathrm{Op}(\sigma)$ given by

$\sigma = \lambda_+\Pi_+ + \lambda_-\Pi_- + \lambda_0\Pi_0$, where, following calculations in [10, 33]

$$\Pi_j = \psi_j\psi_j^*, \quad \psi_0 = \frac{1}{\kappa}\begin{bmatrix} if \\ \zeta \\ -\xi \end{bmatrix}, \quad \psi_\pm = \frac{1}{\rho}\begin{bmatrix} if\xi \pm \kappa\zeta \\ \xi\zeta \pm if\kappa \\ \zeta^2 + f^2 \end{bmatrix}, \quad \lambda_0 = \mu\kappa^2(1+\kappa^2)^{-\frac{1}{2}}, \quad \lambda_\pm = \pm\kappa,$$

with $f \in \mathfrak{S}(f_-, f_+)$, $\kappa = \sqrt{f^2+\xi^2+\zeta^2}$, and $\rho = \kappa\sqrt{2(f^2+\zeta^2)}$ for some nonzero constants μ and $f_\pm$. We verify that $H_\mu = H_0$ when the regularization parameter $\mu = 0$.

The role of the regularization is to replace the infinitely degenerate (flat band) eigenvalue 0 by a topologically trivial band with eigenvalues tending to $\pm\infty$ as $|(\xi,\zeta)| \to \infty$. The choice of the regularization for λ_0 ensure that $\sigma \in S^1_{1,0}$ and is elliptic when $\mu \neq 0$.

As above, we set $\sigma_\pm$ equal to σ with $f(y)$ replaced by $f_\pm$. Defining $\mu_1 := \min\{|\mu|, 1\}$ and $f_0 := \min\{|f_+|, |f_-|\}$, we can set $E_2 := f_0\min\{\mu_1, |\mu| f_0\}$ and $E_1 := -E_2$, so that (H1) is satisfied.

We apply Proposition 2.2.4, with $\mu > 0$ for concreteness. Take $\partial R_3 := \{y^2+\xi^2+\zeta^2 = r^2\} \subset \mathbb{R}^3$, with $r > 0$ sufficiently large so that $|f(y)| \geq f_0$ whenever $|y| \geq r$. The λ_j and ψ_j are differentiable everywhere on ∂R_3, except perhaps where $\rho = 0$. But $\{\rho = 0\} \cap \partial R_3 \subset \{\zeta = 0\} \cap \{y^2+\xi^2 = r^2\}$ has Σ-measure zero, so indeed the regularity requirement is satisfied. Observe that

$$\partial_\xi\psi_0 = \frac{1}{\kappa}\begin{bmatrix} 0 \\ 0 \\ -1 \end{bmatrix} + c_1\psi_0, \quad \partial_\zeta\psi_0 = \frac{1}{\kappa}\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} + c_2\psi_0, \quad \partial_y\psi_0 = \frac{1}{\kappa}\begin{bmatrix} if' \\ 0 \\ 0 \end{bmatrix} + c_3\psi_0,$$

where the c_i are scalar-valued functions. The terms in the integrand of (2.2.12) corresponding to the pair $\{\lambda_0, \lambda_-\}$ are $\Im((\psi_-^*\partial_\xi\psi_0)^*\psi_-^*\partial_\zeta\psi_0) = -\frac{1}{\kappa^2\rho^2}f\kappa(\zeta^2+f^2)$, $\Im((\psi_-^*\partial_\xi\psi_0)^*\psi_-^*\partial_y\psi_0) = \frac{1}{\kappa^2\rho^2}f'\kappa\zeta(\zeta^2+f^2)$, and $\Im((\psi_-^*\partial_\zeta\psi_0)^*\psi_-^*\partial_y\psi_0) = -\frac{1}{\kappa^2\rho^2}f'\kappa\xi(\zeta^2+f^2)$. Thus the contribution to $2\pi\sigma_I$ of $\{\lambda_0, \lambda_-\}$ is

$$
\begin{aligned}
&\frac{i}{2\pi}\int_{\partial R_3} \varepsilon_{ijk}\partial_i\psi_0^*\psi_-\psi_-^*\partial_j\psi_0\nu_k d\Sigma \\
&\quad = \frac{i}{2\pi}\int_{\partial R_3} 2i(\Im((\psi_-^*\partial_\xi\psi_0)^*\psi_-^*\partial_\zeta\psi_0)\nu_y - \Im((\psi_-^*\partial_\xi\psi_0)^*\psi_-^*\partial_y\psi_0)\nu_\zeta \\
&\qquad\qquad\qquad\qquad + \Im((\psi_-^*\partial_\zeta\psi_0)^*\psi_-^*\partial_y\psi_0)\nu_\xi)d\Sigma \\
&\quad = \frac{1}{\pi}\int_{\partial R_3}\frac{\zeta^2+f^2}{\kappa^2\rho^2}(fy+f'\zeta^2+f'\xi^2)d\Sigma = \frac{1}{2\pi}\int_{\partial R_3}\frac{1}{\kappa^4}(fy+f'\zeta^2+f'\xi^2)d\Sigma.
\end{aligned}
$$

Considering the case $f_- < 0 < f_+$, we can without loss of generality take $f(y) = y$ on ∂R_3, so that the integral becomes $\frac{1}{2\pi}\int_{\partial R_3}\frac{1}{\kappa^2}d\Sigma = 2$. One verifies that $\psi_-^*\partial_\xi\psi_+ = \psi_-^*\partial_\zeta\psi_+ = \psi_-^*\partial_y\psi_+ = 0$, meaning there is no contribution to the conductivity from the pair $\{\lambda_+, \lambda_-\}$.

We conclude that $2\pi\sigma_I = 2$, which in practice corresponds to two (observed) eastward-moving asymmetric modes along the equator. A similar calculation shows that $2\pi\sigma_I = 2$ also when $\mu < 0$, so that the conductivity is independent of the regularization parameter $\mu \neq 0$. If instead we assume that $f_+ < 0 < f_-$ (with south pole pointing upwards), then $2\pi\sigma_I = -2$.

2.4 Extension to junction models

Above, we considered models of two 2-dimensional insulators that were joined together along a flat (e.g. $y = 0$) interface. In this subsection, we will generalize the theory to more complicated geometries; see Figure 2.1 for an illustration. Our goal is to describe systems exhibiting surface waves that propagate along the interfaces between the + and − regions with a preferred direction (e.g. moving from left to right). Analogous to (1.0.1), we will define a *junction conductivity* that quantifies the net current associated with these waves at a particular energy. One can define the conductivity so that it measures the contribution from any combination of interfaces (more details below Corollary 2.4.3).

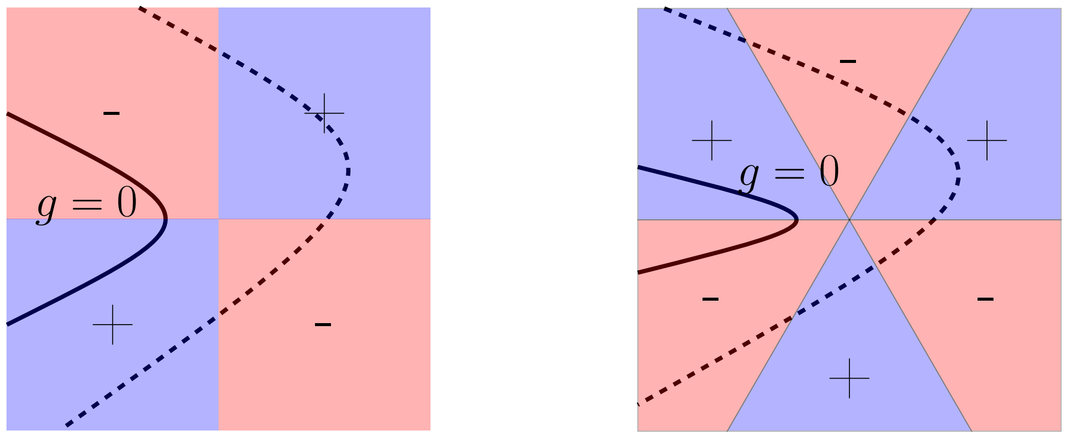

Figure 2.1: Two illustrations of the models considered in Section 2.4. Here, two insulators (labeled by $+$ and $-$) are joined together at a junction. We analyze the asymmetric transport along each interface and through the junction. Two example level curves $\{g = 0\}$ are presented in each case (solid and dashed curves), for some arbitrary choices of g satisfying the appropriate assumptions below. The scale of this picture is much smaller than 1, so that we are not in the region where $g(r, \theta) = r g_\Theta(\theta)$.

The main result of this subsection (Theorem 2.4.8 below) is a bulk-interface correspondence, which equates the conductivity to the difference of two integrals depending only on the associated insulators. In particular, the conductivity does not depend on local properties of the material, such as the way the insulators are joined together at each interface. Theorem 2.4.8 allows for straight-forward evaluations of the conductivity using the previously developed theory for interface models in Sections 2.1–2.3.

The proof of Theorem 2.4.8 requires familiar stability properties of the conductivity, resembling those of the previous subsections. As an alternative approach, we tie the conductivity to a Fredholm index (Theorem 2.4.2), with the latter known to be quantized and invariant with respect to a large class of perturbations. This implies a conservation law (Corollary 2.4.3) showing (among other things) that the currents entering and leaving the junction are the same. We also prove invariance of the junction conductivity with respect to the corresponding density of states (Corollary 2.4.4), semiclassical rescaling (Theorem 2.4.7) and other "continuous" perturbations of the Hamiltonian (Corollary 2.4.5). We conclude the section with applications to a continuum model of twisted bilayer graphene and a 2×2

junction Dirac model.

Let us introduce some notation. As above, the Hamiltonians H act on $\mathcal{H} := L^2(\mathbb{R}^2)\otimes\mathbb{C}^n$. We label the spatial coordinates $(x, y) \in \mathbb{R}^2$ and the corresponding dual variables $(\xi, \zeta) \in \mathbb{R}^2$. Given functions $u \in \mathcal{C}^\infty(\mathbb{R}^2)$ and $A \in \mathcal{C}^\infty(\mathbb{R}^2; \mathbb{C}^{n\times n})$, fixed matrices A_1 and A_2 in $\mathbb{C}^{n\times n}$, and fixed constants $c_1 \le c_2$, we write $A \in \mathfrak{S}(A_1, A_2; c_1, c_2; u)$ to mean that

$$A = \begin{cases} A_1, & u < c_1 \\ A_2, & u > c_2 \end{cases}. \tag{2.4.1}$$

We let $\mathfrak{S}(A_1, A_2; u)$ denote the union of $\mathfrak{S}(A_1, A_2; c_1, c_2; u)$ over all $-\infty < c_1 \le c_2 < \infty$. If $A = A(\alpha)$ is a function of just one variable, then we define $\mathfrak{S}(A_1, A_2; c_1, c_2) := \mathfrak{S}(A_1, A_2; c_1, c_2; \alpha)$ and $\mathfrak{S}(A_1, A_2) := \mathfrak{S}(A_1, A_2; \alpha)$. Note that if $A(x, y) = \chi_A(u(x, y))$ for some $\chi_A \in \mathfrak{S}(A_1, A_2)$, then $A \in \mathfrak{S}(A_1, A_2; u)$.

Let (r, θ) denote the polar coordinates for (x, y). Fix $k \in \mathbb{N}$ and let $\Theta_k \subset \mathbb{T}$ be any set containing $2k$ elements, where $\mathbb{T} := [0, 2\pi)$ is the one-dimensional torus. Let $f_\Theta \in \mathcal{C}^\infty(\mathbb{T})$ such that $f_\Theta(\theta) = 0$ if and only if $\theta \in \Theta_k$, and $f'_\Theta(\theta) \ne 0$ whenever $\theta \in \Theta_k$. This means f_Θ changes sign across every point in Θ_k and is bounded away from 0 for all θ away from Θ_k. Let $f \in \mathcal{C}^\infty(\mathbb{R}^2)$ such that $f(x, y) = f(r, \theta) := r f_\Theta(\theta)$ whenever $r \ge 1$.

As before, we will fix $-\infty < \tilde{E}_1 < \tilde{E}_2 < \infty$ and let $\Phi \in \mathcal{C}_c^\infty(\mathbb{R})$ such that $\Phi \equiv 1$ in $[\tilde{E}_1, \tilde{E}_2]$. We make the following assumption.

(H0') Let $H \in \mathrm{Op}(ES^m_{1,0})$ such that $\Phi(H) \in \mathrm{Op}(S(\langle f(x, y), \xi, \zeta\rangle^{-\infty}))$.

Let $\{\theta_1, \theta_2\} \subset \mathbb{T}$ such that $\theta_1, \theta_2 \notin \Theta_k$. Let $g_\Theta \in \mathcal{C}^\infty(\mathbb{T})$ such that $g_\Theta(\theta) = 0$ if and only if $\theta \in \{\theta_1, \theta_2\}$, and $g'_\Theta(\theta_j) \ne 0$ for $j \in \{1, 2\}$. Let $g \in \mathcal{C}^\infty(\mathbb{R}^2)$ such that $g(x, y) = g(r, \theta) = r g_\Theta(\theta)$ for all $r \ge 1$. Our assumptions on f and g imply the existence of positive constants $C_1 < C_2$ such that

$$C_1\langle x,y\rangle \leq \langle f(x,y), g(x,y)\rangle \leq C_2\langle x,y\rangle. \tag{2.4.2}$$

Moreover, there exists a smooth function $(x_0, y_0) : \mathbb{R} \to \mathbb{R}^2$ with $\lim_{|t|\to\infty} |(x_0(t), y_0(t))| = \infty$ and whose range separates the $xy-$plane into two regions, R_+ and R, such that $g \geq 0$ in R_+. One can for example take a curve contained in $\{g = 0\}$, in which case $(x_0(t), y_0(t)) = (\beta_1 t, \beta_2 t)$ for all $|t|$ sufficiently large, with the constants β_1 and β_2 depending only on $\operatorname{sgn} t$. Our convention is that R_+ be on the *right* side of the curve defined by (x_0, y_0) as t increases. That is, if you were to move along the curve with t increasing, then R_+ would be on your right.

The similarity between (H0) and (H0') naturally implies the following

Lemma 2.4.1. *Suppose H satisfies (H0'), and let $P(x,y) = P \in \mathfrak{S}(0,1;g)$ and $\varphi \in \mathfrak{S}(0,1;\tilde{E}_1,\tilde{E}_2)$. Then $[H,P]\varphi'(H)$ is trace-class. If $\psi \in \mathcal{C}_c^\infty(\tilde{E}_1,\tilde{E}_2)$, then $q(H)[\psi(H),P]$ is trace-class for any polynomial q.*

Proof. Replace (x,y) by $(f(x,y), g(x,y))$ in the proof of Lemma 2.1.1, and use (2.4.2). $\square$

Thus we can define a *junction conductivity* $\sigma_I(H,P,\varphi)$ by (1.0.1), where the switch functions satisfy $\varphi \in \mathfrak{S}(0,1;\tilde{E}_1,\tilde{E}_2)$ as before and $P(x,y) = P \in \mathfrak{S}(0,1;g)$. The stability results from Section 2.1 extend easily to this new setting. For pedagogical purposes, we instead present an alternative method that ties the conductivity to a Fredholm index.

Theorem 2.4.2. *Suppose H satisfies (H0'), and let $P(x,y) = P \in \mathfrak{S}(0,1;g)$ and $\varphi \in \mathfrak{S}(0,1;\tilde{E}_1,\tilde{E}_2)$. Define $U(H) := e^{i2\pi\varphi(H)}$ and let $\bar{P} = \bar{P}(x,y) = \chi(g(x,y)-\alpha)$, where $\chi : \mathbb{R} \to \mathbb{R}$ is the Heavyside step function and $\alpha \in \mathbb{R}$. Then $\bar{P}U(H)\bar{P}$ is a Fredholm operator on the range of $\bar{P}$, with*

$$2\pi\sigma_I(H,P,\varphi) = \operatorname{Index}(\bar{P}U(H)\bar{P}).$$

Proof. We will prove that

$$2\pi\sigma_I(H,P,\varphi) = \mathrm{Tr}[U,P]U^* = \mathrm{Tr}[U,\bar{P}]U^* = \mathrm{Index}(\bar{P}U\bar{P}), \tag{2.4.3}$$

where we use the shorthand $U := U(H)$.

We begin by proving the first equality in (2.4.3). Let $V := U - I$, and observe that $V \in \mathcal{C}_c^\infty(\{\Phi = 1\}^\circ)$. We have

$$\mathrm{Tr}[U,P]U^* = \mathrm{Tr}[V,P]U^* = \mathrm{Tr}[V,P]V^* + \mathrm{Tr}[V,P].$$

Using that $[(z-H)^{-1},P] = (z-H)^{-1}[H,P](z-H)^{-1}$, the Helffer-Sjöstrand formula (A.1.6) and cyclicity of the trace [57] imply that

$$\mathrm{Tr}[V,P]V^* = \mathrm{Tr}\Big(-\frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{V}(z)[H,P](z-H)^{-2}d^2z V^*(H)\Big).$$

After integrating by parts in ∂ and using that $\partial\tilde{V} = \tilde{V'}$ for some almost analytic extension $\tilde{V'}$ of V', we see that

$$\begin{aligned}\mathrm{Tr}[V,P]V^* = \mathrm{Tr}[H,P]V'V^* &= 2\pi\sigma_I(H,P) - \mathrm{Tr}\,2\pi i[H,P]\varphi'U \\ &= 2\pi\sigma_I(H,P,\varphi) - \mathrm{Tr}[H,P]V'.\end{aligned} \tag{2.4.4}$$

We have thus shown that

$$\mathrm{Tr}[U,P]U^* = 2\pi\sigma_I(H,P) - \mathrm{Tr}[H,P]V' + \mathrm{Tr}[V,P].$$

By the same logic used in (2.4.4), we obtain that $\mathrm{Tr}[H,P]V' = \mathrm{Tr}[H,P]V'\Phi = \mathrm{Tr}[V,P]\Phi$, hence

$$\operatorname{Tr}[U, P]U^* = 2\pi\sigma_I(H, P, \varphi) + \operatorname{Tr}[V, P](1 - \Phi).$$

Again using cyclicity of the trace, this means

$$\operatorname{Tr}[U, P]U^* = 2\pi\sigma_I(H, P, \varphi) + \operatorname{Tr}\Psi_1[V, P]\Psi_2,$$

for some $\Psi_j = \psi_j(H)$, where $\psi_j \in \mathcal{C}^\infty(\mathbb{R})$ vanishes on $\operatorname{supp}(V)$. The first equality in (2.4.3) follows.

We now prove the second equality of (2.4.3). Let $\chi(x, y) = \chi_1(g(x, y))$ where $\chi_1 \in \mathcal{C}_c^\infty$ such that $\chi(\bar{P} - P) = \bar{P} - P$. Then

$$[U, \bar{P} - P]U^* = [V, \bar{P} - P]U^* = V\chi(\bar{P} - P)U^* - (\bar{P} - P)\chi VU^*$$

is trace class, as $V\chi$ and χV are both trace-class by the ΨDO calculus with $P - P_1$ and U^* bounded. Since we know that $[U, P]U^*$ is trace-class, this proves that

$$[U, \bar{P}]U^* = [U, \bar{P} - P]U^* + [U, P]U^*$$

is trace-class. Now,

$$\operatorname{Tr}[U, \bar{P} - P]U^* = \operatorname{Tr}V\chi(\bar{P} - P)U^* - \operatorname{Tr}(\bar{P} - P)\chi VU^*,$$

with

$$\operatorname{Tr}V\chi(\bar{P} - P)U^* = \operatorname{Tr}(\bar{P} - P)U^*V\chi$$

and

$$\operatorname{Tr}(\bar{P}-P)\chi V U^* = \operatorname{Tr}\chi(\bar{P}-P)\chi V U^* = \operatorname{Tr}(\bar{P}-P)\chi V U^*\chi = \operatorname{Tr}(\bar{P}-P)V U^*\chi.$$

Since $[V, U^*] = 0$, we have proven that $\operatorname{Tr}[U, \bar{P}-P]U^* = 0$, which verifies the second equality of (2.4.3).

Finally, the last equality of (2.4.3) follows immediately from [6, Proposition 2.4] and the fact that $[U, \bar{P}]U^*$ is trace-class. □

Theorem 2.4.2 is a powerful result with many implications. For example, we immediately have the following three corollaries.

Corollary 2.4.3. *Suppose H satisfies (H0'), $P, P_1 \in \mathfrak{S}(0, 1; g(x, y))$ and $\varphi \in \mathfrak{S}(0, 1; \tilde{E}_1, \tilde{E}_2)$. Then*

$$\sigma_I(H, P, \varphi) = \sigma_I(H, P_1, \varphi).$$

Proof. Applying Theorem 2.4.2, we have $2\pi\sigma_I(H, P, \varphi) = \operatorname{Index}(\bar{P}U(H)\bar{P}) = 2\pi\sigma_I(H, P_1, \varphi)$. □

For an intuitive explanation of the above corollary, recall that our model is of two types of materials ($+$ and $-$) that are smoothly glued together at a junction. See Figure 2.1 for two examples, where we assume for concreteness that P transitions from 0 to 1 in the vicinity of $\{g = 0\}$. The solid curve (in both panels) can see only one transition ($+$ to $-$ and $-$ to $+$ in the left and right panels, respectively), while the dashed level curves contain multiple transitions ($+ \to - \to + \to -$ for the left panel and $- \to + \to - \to + \to - \to +$ for the right panel). As expected, the conductivity only cares about the "starting" and "ending" topology along the level curve and is unaffected by oscillations in between. Observe that Corollary 2.4.3 describes a conservation law, as the solid and dashed curves respectively measure the conductivity entering and leaving the junction.

Corollary 2.4.4. *Suppose H satisfies (H0'), and let $P(x,y) = P \in \mathfrak{S}(0,1;g)$ and $\varphi, \varphi_1 \in \mathfrak{S}(0,1;\tilde{E}_1,\tilde{E}_2)$. Then*

$$\sigma_I(H,P,\varphi) = \sigma_I(H,P,\varphi_1).$$

Proof. For $\mu \in [0,1]$, define $\varphi_\mu := \varphi + \mu(\varphi_1 - \varphi)$. Theorem 2.4.2 implies that $\sigma_I(H,P,\varphi'_\mu) = \mathrm{Index}(\bar{P}U_\mu\bar{P})$ for all $\mu \in [0,1]$, where $U_\mu := e^{i2\pi\varphi_\mu(H)}$. With $V_\mu := U_\mu - I$, the Helffer-Sjöstrand formula (A.1.6) implies

$$U_{\mu_2} - U_{\mu_1} = V_{\mu_2} - V_{\mu_1} = -\frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}(\tilde{V}_{\mu_2}(z) - \tilde{V}_{\mu_1}(z))(z-H)^{-1}d^2z.$$

Since $|\bar{\partial}(\tilde{V}_{\mu_2}(z) - \tilde{V}_{\mu_1}(z))| \le C|\mu_2 - \mu_1|$ uniformly in $\mu_1,\mu_2 \in [0,1]$ and $z \in \mathbb{C}$, it follows that $\left\|U_{\mu_2} - U_{\mu_1}\right\| \to 0$ as $\mu_2 - \mu_1 \to 0$. Therefore, by [55, Theorem 19.1.5], $\mathrm{Index}(\bar{P}U_\mu\bar{P})$ is independent of $\mu \in [0,1]$, and the result is complete. □

Corollary 2.4.5. *Let $H \in \mathrm{Op}(ES^m_{1,0})$ and $W \in \mathrm{Op}(S^m_{1,0})$ such that $H^{(\mu)} := H + \mu W$ satisfies (H0') for all $\mu \in [0,1]$. Let $P(x,y) = P \in \mathfrak{S}(0,1;g)$ and $\varphi \in \mathfrak{S}(0,1;\tilde{E}_1,\tilde{E}_2)$. Then $\sigma_I(H^{(1)},P,\varphi) = \sigma_I(H,P,\varphi)$.*

As before, in the following proofs we write $A \in \mathrm{Op}(\mu S(\mathfrak{m}))$ to mean that $A = \mathrm{Op}(a)$ with $a \in S(\mathfrak{m})$ for all μ and $|\partial^\alpha a| \le C_\alpha \mu \mathfrak{m}$ uniformly in μ.

Proof. We use the shorthand $\sigma_I(H^{(\mu)}) := \sigma_I(H^{(\mu)},P,\varphi)$. By definition, $\Phi \in \mathcal{C}^\infty_c(E_1,E_2)$ satisfies $\varphi'\Phi = \varphi'$. We see that

$$\begin{aligned}&\sigma_I(H^{(\mu_2)}) - \sigma_I(H^{(\mu_1)}) = \\ &\qquad \operatorname{Tr} i[H^{(\mu_2)},P](\varphi'(H^{(\mu_2)}) - \varphi'(H^{(\mu_1)})) + (\mu_2 - \mu_1)\operatorname{Tr} i[W,P]\varphi'(H^{(\mu_1)}),\end{aligned}$$

with

$$\varphi'(H^{(\mu_2)}) - \varphi'(H^{(\mu_1)}) = \frac{1}{\pi}(\mu_2 - \mu_1) \int_{\mathbb{C}} \bar{\partial}\tilde{\varphi}'(z)(z - H^{(\mu_2)})^{-1} W (z - H^{(\mu_1)})^{-1} d^2 z$$

by the Helffer-Sjöstrand formula (A.1.6). Observe that

$$\varphi'(H^{(\mu_2)}) - \varphi'(H^{(\mu_1)}) \in \mathrm{Op}(|\mu_2 - \mu_1| S(\langle x, y, \xi, \zeta\rangle^m)) \cap \mathrm{Op}(S(\langle f(x,y), \xi, \zeta\rangle^{-\infty})),$$

and thus

$$\varphi'(H^{(\mu_2)}) - \varphi'(H^{(\mu_1)}) \in \mathrm{Op}(|\mu_2 - \mu_1|^{1/2} S(\langle f(x,y), \xi, \zeta\rangle^{-\infty}))$$

by interpolation. Since $[H^{(\mu_2)}, P] \in \mathrm{Op}(S(\langle x, y, \xi, \zeta\rangle^m \langle g(x,y)\rangle^{-\infty}))$, the composition calculus implies that

$$|\operatorname{Tr} i[H^{(\mu_2)}, P](\varphi'(H^{(\mu_2)}) - \varphi'(H^{(\mu_1)}))| \leq C|\mu_2 - \mu_1|^{1/2}.$$

Since $|\operatorname{Tr} i[W, P]\varphi'(H^{(\mu_1)})| \leq C$ independent of μ_2, we have shown that $\mu \mapsto \sigma_I(H^{(\mu)})$ is continuous on $\mu \in [0,1]$. But Theorem 2.4.2 implies that $2\pi\sigma_I(H^{(\mu)})$ is equal to an (integer-valued) Fredholm index for all μ, and thus $\sigma_I(H^{(\mu)})$ is independent of $\mu \in [0,1]$. $\square$

Analogous to (H1), we now introduce the following class of symbols.

(H1') Let $H = \mathrm{Op}(\sigma)$ with $\sigma \in ES^m_{1,0}$. Suppose there exist symbols $\sigma_\pm \in S^m_{1,0}$ independent of (x, y) with no spectrum in the open interval (E_1, E_2), such that $\sigma = \sigma_\pm$ whenever $\pm f(x, y) > 0$ is sufficiently large.

We then have

Proposition 2.4.6. *Suppose* $H = \mathrm{Op}(\sigma)$ *satisfies (H1') and* $\Phi \in \mathcal{C}_c^\infty(E_1, E_2)$*. Define* $H_h := \mathrm{Op}_h(\sigma)$ *for* $h \in (0,1]$*. Then* $\Phi(H_h) \in \mathrm{Op}_h(S(\langle f(x,y), \xi, \zeta\rangle^{-\infty}))$*.*

Proof. See the proof of Proposition 2.1.10. $\square$

Proposition 2.4.6 proves that the class (H1') is a subset of (H0'). We now show that under (H1'), the interface conductivity is stable with respect to semi-classical rescaling.

Theorem 2.4.7. *Suppose* $H = \mathrm{Op}(\sigma)$ *satisfies (H1'), and define* $H_h := \mathrm{Op}_h(\sigma)$*. Let* $P(x,y) = P \in \mathfrak{S}(0,1;g)$ *and* $\varphi \in \mathfrak{S}(0,1;E_1,E_2)$*. Then* $\sigma_I(H_h, P, \varphi) = \sigma_I(H, P, \varphi)$ *for all* $h \in (0,1]$*.*

Proof. For $h \in (0,1]$, define $U_h := e^{i2\pi\varphi(H_h)}$. Proposition 2.4.6 and Theorem 2.4.2 imply that $2\pi\sigma_I(H_h, P, \varphi) = \mathrm{Index}(\bar{P}U_h\bar{P})$ for all $h \in (0,1]$. It thus suffices to show that for any fixed $h \in (0,1]$, $\mathrm{Index}(\bar{P}U_{h'}\bar{P})$ is constant over h' in an open neighborhood of h. Using the Helffer-Sjöstrand formula (A.1.6), we write

$$U_{h'} - U_h = \frac{1}{\pi}\int_{\mathbb{R}} \bar{\partial}\tilde{V}(z)(z - H_{h'})^{-1}(H_{h'} - H_h)(z - H_h)^{-1} d^2 z.$$

Since $\left\|(z - H_{h'})^{-1}\right\| \le |\Im z|^{-1}$ and $H_{h'} - H_h \in \mathrm{Op}(|h' - h| S(\langle \xi, \zeta\rangle^m))$ with $(z - H_h)^{-1} \in \mathrm{Op}(S(\langle \xi, \zeta\rangle^{-m}))$ for all $\Im z \neq 0$ (with bounds growing at most algebraically in $|\Im z|^{-1}$), the rapid decay of $\bar{\partial}\tilde{V}(z)$ near the real axis implies that $\|U_{h'} - U_h\| \le C|h' - h|$. The result then follows from [55, Theorem 19.1.5]. $\square$

2.4.1 Bulk-interface correspondence

As in Section 2.2, the above results allow for an accessible formula for $\sigma_I(H, P, \varphi)$. In particular, we will prove a bulk-interface correspondence, extending Corollary 2.2.2 to the junction setting.

For $(t,\xi,\zeta)\in\mathbb{R}^3$, define

$$\tau(t,\xi,\zeta) := \sigma(x_0(t), y_0(t), \xi, \zeta), \qquad \tau_z := z-\tau, \tag{2.4.5}$$

where we recall the definition of (x_0, y_0) below (2.4.2). By (H1'), there exist $t_0 > 0$ and symbols $\tau_\pm \in \{\sigma_+, \sigma_-\}$ such that $\tau(t,\xi,\zeta) = \tau_\pm(\xi,\zeta)$ whenever $\pm t \geq t_0$.

Theorem 2.4.8. *Suppose H satisfies (H1'), $P(x,y) = P \in \mathfrak{S}(0,1;g)$ and $\varphi \in \mathfrak{S}(0,1;E_1,E_2)$. Let $\alpha \in (E_1,E_2)$ and define $\tau_{\pm,z} := z - \tau_\pm$ with $z = \alpha + i\omega$. Then*

$$2\pi\sigma_I(H,P,\varphi) = \frac{i}{8\pi^2}(I_+ - I_-), \qquad I_\pm = \int_{\mathbb{R}^3} \operatorname{tr}[\tau_{\pm,z}^{-1}\partial_\xi \tau_{\pm,z}, \tau_{\pm,z}^{-1}\partial_\zeta \tau_{\pm,z}]\tau_{\pm,z}^{-1} d\omega d\xi d\zeta.$$

As with Theorem 2.2.1, we will expand $\sigma_I(H_h, P, \varphi)$ in the semiclassical parameter h and apply Theorem 2.4.7 to eliminate terms that are not $O(1)$.

Proof. By Theorem 2.4.4, $\sigma_I(H,P,\varphi)$ is independent of $\varphi \in \mathfrak{S}(0,1;E_1,E_2)$, thus we can take $\varphi' \in \mathcal{C}_c^\infty(\alpha_0,\alpha)$ for some $\alpha_0 > E_1$. We will use the shorthand $\sigma_I := \sigma_I(H,P,\varphi)$.

Let $\operatorname{Op}_h \nu_h := \varphi'(H_h)$. By Proposition A.3.3, we have

$$\nu_h + \frac{1}{\pi}\int_{\mathbb{C}} \bar\partial\tilde{\varphi}'(z)\tilde{q}_{z,h} d^2z \in S^{-3/2}(\langle f(x,y),\xi,\zeta\rangle^{-\infty}),$$

where

$$\tilde{q}_{z,h} = \sigma_z^{-1} + \frac{ih}{2}\{\sigma_z^{-1},\sigma_z\}\sigma_z^{-1}, \qquad \{a,b\} := \partial_\xi a\partial_x b + \partial_\zeta a \partial_y b - \partial_x a\partial_\xi b - \partial_y a \partial_\zeta b$$

and $\sigma_z := z - \sigma$. With $\operatorname{Op}_h(\kappa_h) := [H_h, P]$, we have that

$$\kappa_h + ihk_1 - \frac{h^2}{4}k_2 \in S^{-3}(\langle g(x,y)\rangle^{-\infty}\langle \xi,\zeta\rangle^m),$$

where

$$k_1 := \partial_\xi \sigma \partial_x P + \partial_\zeta \sigma \partial_y P, \qquad k_2 := \partial_{\xi\xi}\sigma \partial_{xx} P + 2\partial_{\xi\zeta}\sigma\partial_{xy}P + \partial_{\zeta\zeta}\sigma\partial_{yy}P. \tag{2.4.6}$$

Since $\nu_h \in S(\langle f(x,y),\xi,\zeta\rangle^{-\infty})$ and $\kappa_h \in S^{-1}(\langle g(x,y)\rangle^{-\infty}\langle \xi,\zeta\rangle^m)$, the composition calculus implies that

$$\kappa_h \sharp_h \nu_h - \kappa_h \nu_h + \frac{ih}{2}\{\kappa_h,\nu_h\} \in S^{-3}(\langle x,y,\xi,\zeta\rangle^{-\infty}),$$

with S^{-3} (rather than S^{-2}) above because κ_h is $O(h)$ in $S(\langle g(x,y)\rangle^{-\infty}\langle\xi,\zeta\rangle^m)$. Therefore,

$$\sigma_I = \frac{i}{(2\pi h)^2}\operatorname{tr}\int_{\mathbb{R}^4}\kappa_h\sharp_h\nu_h dR_4 = \frac{i}{(2\pi h)^2}\operatorname{tr}\int_{\mathbb{R}^4}\Big(\kappa_h\nu_h - \frac{ih}{2}\{\kappa_h,\nu_h\}\Big)dR_4 + o(1)$$

as $h \to 0$, with $dR_4 := dxdyd\xi d\zeta$. Since

$$\kappa_h\nu_h = (ihk_1 - \frac{h^2}{4}k_2)\frac{1}{\pi}\int_{\mathbb{C}}\bar\partial\tilde{\varphi}'(z)\Big(\sigma_z^{-1} + \frac{ih}{2}\{\sigma_z^{-1},\sigma_z\}\sigma_z^{-1}\Big)d^2z + h^{5/2}a_h$$

for some $a_h \in S(\langle x,y,\xi,\zeta\rangle^{-\infty})$ and

$$\{\kappa_h,\nu_h\} = \Big\{ihk_1, \frac{1}{\pi}\int_{\mathbb{C}}\bar\partial\tilde{\varphi}'(z)\sigma_z^{-1}d^2z\Big\} + h^2 b_h, \qquad b_h \in S(\langle x,y,\xi,\zeta\rangle^{-\infty}),$$

it follows that

$$\begin{aligned}\sigma_I = \frac{i}{(2\pi h)^2}\frac{1}{\pi}\operatorname{tr}\int_{\mathbb{R}^4}\int_{\mathbb{C}}\bar\partial\tilde{\varphi}'(z)\Big(&ihk_1\sigma_z^{-1} - \frac{h^2}{2}k_1\{\sigma_z^{-1},\sigma_z\}\sigma_z^{-1}\\ &- \frac{h^2}{4}k_2\sigma_z^{-1} + \frac{h^2}{2}\{k_1,\sigma_z^{-1}\}\Big)d^2z dR_4 + o(1)\end{aligned}$$

as $h \to 0$. Since σ_I is independent of h, it follows that the $O(h^{-1})$ term above vanishes, and thus

$$\sigma_I = \frac{i}{(2\pi)^3}\operatorname{tr}\int_{\mathbb{R}^4}\int_{\mathbb{C}} \bar\partial\tilde{\varphi}'(z)\Big(- k_1\sigma_z^{-1}\{\sigma_z,\sigma_z^{-1}\} - \frac{1}{2}k_2\sigma_z^{-1} + \{k_1,\sigma_z^{-1}\}\Big)d^2z dR_4.$$

Observe that whenever $\langle f(x,y),\xi,\zeta\rangle$ is sufficiently large, $z\mapsto\sigma_z^{-1}$ is holomorphic and thus the above integral over z vanishes (this is verified via an integration by parts in $\bar\partial$). Using that k_1 and k_2 vanish whenever $\langle g(x,y)\rangle$ is sufficiently large, we can replace the above integration limit $\mathbb{R}^4$ by a sufficiently large rectangle $B := B_{xy}\times B_{\xi\zeta}\subset\mathbb{R}^2\times\mathbb{R}^2$. We require that B contain all points $(x_0(t),y_0(t),\xi,\zeta)$ for which $\sigma(x_0(t),y_0(t),\xi,\zeta)$ has an eigenvalue of α. Moreover, assume that B_{xy} contains $(x_0(t_0),y_0(t_0))$ and $(x_0(-t_0),y_0(-t_0))$, where we recall the respective definitions of t_0 and (x_0,y_0) above Theorem 2.4.8 and below (2.4.2).

At this point, $\{k_1,\sigma_z^{-1}\}$ can be written in divergence form and the corresponding term converted (via integration by parts in (x,y,ξ,ζ)) to an integral over the surface ∂B. An integration by parts in $\bar\partial$ then reveals that the contribution of this term vanishes. Thus we are left with

$$\sigma_I = -\frac{i}{(2\pi)^3}\operatorname{tr}\int_B\int_{\mathbb{C}} \bar\partial\tilde{\varphi}'(z)\Big(k_1\sigma_z^{-1}\{\sigma_z,\sigma_z^{-1}\} + \frac{1}{2}k_2\sigma_z^{-1}\Big)d^2z dR_4. \tag{2.4.7}$$

We now simplify the first term above. Integrating by parts in $\bar\partial$ with $z =: \lambda + i\omega$, we see that

$$\begin{aligned}\sigma_{I,1} &:= \frac{-i}{(2\pi)^3}\operatorname{tr}\int_B\int_{\mathbb{C}} \bar\partial\tilde{\varphi}'(z)k_1\sigma_z^{-1}\{\sigma_z,\sigma_z^{-1}\}d^2z dR_4\\ &= \frac{-1}{2(2\pi)^3}\operatorname{tr}\int_B\int_{\alpha_0}^{\alpha}\varphi'(\lambda)k_1\sigma_z^{-1}\{\sigma_z,\sigma_z^{-1}\}\Big|_{\omega=0^-}^{\omega=0^+} d\lambda dR_4.\end{aligned}$$

Let $\mathcal{L} := \{x_0(t),y_0(t) : t\in\mathbb{R}\}$ be the range of (x_0,y_0). For simplicity, assume that $\mathcal{L}\subset$

$g^{-1}(0)$. By cyclicity of the trace and recalling the definition (2.4.6) of k_1, it follows that

$$\operatorname{tr} k_1\{\sigma_z^{-1},\sigma_z\}\sigma_z^{-1} = -\operatorname{tr}(\partial_x P\partial_\xi\sigma_z\{\sigma_z^{-1},\sigma_z\}_{\zeta,y} + \partial_y P\partial_\zeta\sigma_z\{\sigma_z^{-1},\sigma_z\}_{\xi,x})\sigma_z^{-1},$$

where we have defined $\{a,b\}_{\alpha,\beta} := \partial_\alpha a\partial_\beta b - \partial_\beta a\partial_\alpha b$ and used the fact that $(\partial_\xi\sigma,\partial_\zeta\sigma) = -(\partial_\xi\sigma_z,\partial_\zeta\sigma_z)$. Integrating by parts in x (first term) and y (second term), we obtain

$$\begin{aligned}
\sigma_{I,1} = &-\frac{1}{2(2\pi)^3}\operatorname{tr}\int_B\int_{\alpha_0}^{\alpha}\varphi'(\lambda)P\Big(\partial_x(\partial_\xi\sigma_z\{\sigma_z^{-1},\sigma_z\}_{\zeta,y}\sigma_z^{-1}) \\
&\qquad + \partial_y(\partial_\zeta\sigma_z\{\sigma_z^{-1},\sigma_z\}_{\xi,x}\sigma_z^{-1})\Big)\Big|_{\omega=0^-}^{\omega=0^+} d\lambda dR_4 \\
&+ \frac{1}{2(2\pi)^3}\operatorname{tr}\int_{B_{\xi\zeta}}\int_{B_{xy}\cap\mathcal{L}}\int_{\alpha_0}^{\alpha}\varphi'(\lambda)(\partial_\xi\sigma_z\{\sigma_z^{-1},\sigma_z\}_{\zeta,y}\nu_x \\
&\qquad + \partial_\zeta\sigma_z\{\sigma_z^{-1},\sigma_z\}_{\xi,x}\nu_y)\sigma_z^{-1}\Big|_{\omega=0^-}^{\omega=0^+} d\lambda d\ell dR_2 \\
=:&\ \sigma_{I,10} + \sigma_{I,11},
\end{aligned}$$

where $dR_2 := d\xi d\zeta$ and $d\ell$ is the integration measure on $\mathcal{L}$. Here, ν is the unit vector (outwardly) normal to the surface $\partial(\{g(x,y) \le 0\} \cap B_{xy})$. Note that the other surface terms do not contribute; over $(\partial(\{g(x,y) \le 0\} \cap B_{xy})) \setminus (B_{xy} \cap \mathcal{L})$, either $P = 0$ or the map $z \mapsto \sigma_z^{-1}$ is holomorphic and thus the difference between $\omega = 0^+$ and $\omega = 0^-$ vanishes.

We now verify that the volume term $\sigma_{I,10}$ vanishes. First, observe that

$$\int_B\int_{\alpha_0}^{\alpha}\varphi'(\lambda)P\Big(\partial_\xi(\partial_x\sigma_z\{\sigma_z^{-1},\sigma_z\}_{\zeta,y}\sigma_z^{-1}) + \partial_\zeta(\partial_y\sigma_z\{\sigma_z^{-1},\sigma_z\}_{\xi,x}\sigma_z^{-1})\Big)\Big|_{\omega=0^-}^{\omega=0^+} d\lambda dR_4 = 0,$$

as we can use the fact that P is independent of (ξ,ζ) to integrate the above left-hand side by parts in ξ (first term) and ζ (second term) to obtain integrals over $\partial B_{\xi\zeta}$, over which

$z \mapsto \sigma_z^{-1}$ is holomorphic. Therefore,

$$\sigma_{I,10} = -\frac{1}{2(2\pi)^3} \int_B \int_{\alpha_0}^{\alpha} \varphi'(\lambda) P \operatorname{tr} \Big(\partial_x(\partial_\xi \sigma_z \{\sigma_z^{-1}, \sigma_z\}_{\zeta,y} \sigma_z^{-1}) + \partial_y(\partial_\zeta \sigma_z \{\sigma_z^{-1}, \sigma_z\}_{\xi,x} \sigma_z^{-1})$$
$$- \partial_\xi(\partial_x \sigma_z \{\sigma_z^{-1}, \sigma_z\}_{\zeta,y} \sigma_z^{-1}) - \partial_\zeta(\partial_y \sigma_z \{\sigma_z^{-1}, \sigma_z\}_{\xi,x} \sigma_z^{-1}) \Big) \Big|_{\omega=0^-}^{\omega=0^+} d\lambda dR_4.$$

A brute force calculation reveals that the above trace vanishes, and thus indeed $\sigma_{I,10} = 0$.

For $\sigma_{I,11}$, we again use cyclicity of the trace to verify that

$$\operatorname{tr}(\partial_\xi \sigma_z \{\sigma_z^{-1}, \sigma_z\}_{\zeta,y} \sigma_z^{-1} \nu_x + \partial_\zeta \sigma_z \{\sigma_z^{-1}, \sigma_z\}_{\xi,x} \sigma_z^{-1} \nu_y)$$
$$= \operatorname{tr}((\nu_x \partial_y \sigma_z - \nu_y \partial_x \sigma_z) \{\sigma_z^{-1}, \sigma_z\}_{\xi,\zeta} \sigma_z^{-1}).$$

We recognize the first factor on the above right-hand side as the derivative of σ_z in the direction of $\mathcal{L}$ (with t increasing). Recalling the definition of τ in (2.4.5), we see that

$$\partial_t \tau(t,\xi,\zeta) = x_0'(t) \partial_x \sigma(x_0(t), y_0(t), \xi, \zeta) + y_0'(t) \partial_y \sigma(x_0(t), y_0(t), \xi, \zeta),$$
$$\partial_\xi \tau(t,\xi,\zeta) = \partial_\xi \sigma(x_0(t), y_0(t), \xi, \zeta), \qquad \partial_\zeta \tau(t,\xi,\zeta) = \partial_\zeta \sigma(x_0(t), y_0(t), \xi, \zeta),$$

with $(x_0', y_0') = N(-\nu_y, \nu_x)$ and $d\ell = N dt$, where $N := \sqrt{(x_0'(t))^2 + (y_0'(t))^2}$. We conclude that

$$\sigma_{I,1} = \frac{1}{16\pi^3} \operatorname{tr} \int_R \int_{[\alpha_0,\alpha]} \varphi'(\lambda) \partial_t \tau_z \{\tau_z^{-1}, \tau_z\}_{\xi,\zeta} \tau_z^{-1} \Big|_{\omega=0^-}^{\omega=0^+} d\lambda dR_3, \tag{2.4.8}$$

where $R = (t_1, t_2) \times B_{\xi\zeta}$ with $t_1 = \inf\{t : (x_0(t), y_0(t)) \in B_{xy}\}$ and $t_2 = \sup\{t : (x_0(t), y_0(t)) \in B_{xy}\}$, and $dR_3 := dt d\xi d\zeta$.

We next eliminate φ' from (2.4.8). Since $\partial_t \tau_z \{\tau_z^{-1}, \tau_z\}_{\xi,\zeta} \tau_z^{-1} \to 0$ as $|\omega| \to \infty$, we have

$$\partial_t \tau_z \{\tau_z^{-1}, \tau_z\}_{\xi,\zeta} \tau_z^{-1} \Big|_{\omega=0^-}^{\omega=0^+} = -\int_{-\infty}^{+\infty} \partial_\omega (\partial_t \tau_z \{\tau_z^{-1}, \tau_z\}_{\xi,\zeta} \tau_z^{-1}) d\omega.$$

Cyclicity of the trace and the fact that $\partial_\omega \tau_z = i$ imply that

$$\operatorname{tr} \partial_\omega(\partial_t \tau_z \{\tau_z^{-1}, \tau_z\}_{\xi,\zeta} \tau_z^{-1}) = -i \operatorname{tr} \varepsilon_{ijk} \partial_k (\tau_z^{-1} \partial_i \tau_z \tau_z^{-1} \partial_j \tau_z \tau_z^{-1}), \tag{2.4.9}$$

where ε_{ijk} is the anti-symmetric tensor with $\varepsilon_{123} = 1$, and the variables are identified by $(1, 2, 3) = (\xi, \zeta, t)$. Pulling ∂_k out of the integral over ω and integrating by parts, we get

$$\operatorname{tr} \int_R \partial_t \tau_z \{\tau_z^{-1}, \tau_z\}_{\xi,\zeta} \tau_z^{-1} \Big|_{\omega=0^-}^{\omega=0^+} dR_3 = i \int_{\partial R} \int_{-\infty}^{+\infty} \Theta d\omega d\Sigma,$$

where

$$\Theta := \operatorname{tr} \varepsilon_{ijk} \tau_z^{-1} \partial_i \tau_z \tau_z^{-1} \partial_j \tau_z \tau_z^{-1} \nu_k,$$

and ν is the outward unit normal vector to the surface ∂R with Σ the Euclidean surface measure in $\mathbb{R}^3$. Thus we have shown that

$$\sigma_{I,1} = \frac{i}{16\pi^3} \int_{[\alpha_0,\alpha]} \varphi'(\lambda) \int_{\partial R} \int_{-\infty}^{+\infty} \Theta d\omega d\Sigma d\lambda.$$

Integrating by parts in λ, we obtain

$$\sigma_{I,1} = \frac{i}{16\pi^3} \int_{\partial R} \int_{-\infty}^{+\infty} \Theta d\omega d\Sigma,$$

with now $z = \alpha + i\omega$ in the above integrand (and from now on). The fact that only the boundary term survives follows from analyticity of Θ in z over the region of integration (so that $\partial_\lambda \Theta = -i\partial_\omega \Theta$).

Recall that $R = (-t_0, t_0) \times (-M, M)^2$, where $M > 0$ can be chosen as large as necessary. Observe that $|\Theta| \le C\langle\omega\rangle^{-3}$ and $|\Theta| \le C\langle\xi,\zeta\rangle^{-m-2}$ uniformly in $(t, \xi, \zeta) \in \partial R$ and $M > 0$ sufficiently large, hence $|\Theta| \le C\langle\omega\rangle^{-3/2}\langle\xi,\zeta\rangle^{-\frac{m+2}{2}}$ by interpolation. It follows that

$\int_{-\infty}^{+\infty} |\Theta| d\omega \leq C\langle \xi, \zeta \rangle^{-\frac{m+2}{2}}$. Therefore, sending $M \to \infty$, we see that the contributions to $\sigma_{I,1}$ from the sides of ∂R with normal vector in the ξ and ζ directions vanish. Indeed, the area of these surfaces is proportional to M, with the maximum of the integrand bounded by $CM^{-1-m/2}$. Thus we are left with integrals over the sides corresponding to $t = \pm t_0$, over which $\tau(t, \xi, \zeta) = \tau_{\pm}(\xi, \zeta)$. As a consequence, $\sigma_{I,1} = \frac{i}{16\pi^3}(I_+ - I_-)$.

Recalling (2.4.7), it remains to show that

$$\sigma_{I,2} := -\frac{i}{2(2\pi)^3} \operatorname{tr} \int_{\mathbb{R}^4} k_2 \int_{\mathbb{C}} \bar{\partial}\tilde{\varphi}'(z)\sigma_z^{-1} d^2z dR_4 = 0. \tag{2.4.10}$$

Define $P_\varepsilon(x, y) := P(\varepsilon(x-\tilde{x}, y-\tilde{y}))$, where $(\tilde{x}, \tilde{y}) \in \mathbb{R}^2$ is chosen such that $P_\varepsilon(x_0(t), y_0(t)) = 1$ for all $\varepsilon > 0$ and $t \in \mathbb{R}$. Corollary 2.4.3 implies that $\sigma_I(H, P_\varepsilon)$ is independent of ε, while $\sigma_{I,1}$ is independent of ε since $I_\pm$ are. It follows that $\sigma_{I,2}$ must also be independent of $\varepsilon > 0$.

We will thus replace P by P_ε and show that $\sigma_{I,2} \to 0$ as $\varepsilon \downarrow 0$. As stated in the paragraph below (2.2.4), the integral over $\mathbb{C}$ in (2.4.10) vanishes whenever $\langle f(x, y), \xi, \zeta \rangle$ is sufficiently large (uniformly in ε). From the definition (2.4.6), it follows that $k_2 = \varepsilon^2 \tilde{k}_{2,\varepsilon}$, where $\tilde{k}_{2,\varepsilon}$ vanishes whenever $\langle \varepsilon g(x-\tilde{x}, y-\tilde{y}) \rangle$ is sufficiently large. We conclude that there exist positive constants M_1 and M_2 such that

$$|\sigma_{I,2}| \leq C\varepsilon^2 \mathrm{Vol}(\{\langle f(x, y) \rangle \leq M_1\} \cap \{\langle \varepsilon g(x - \tilde{x}, y - \tilde{y}) \rangle \leq M_2\}) \leq C\varepsilon,$$

with the above volume taken in the xy-plane. We have thus shown that $\sigma_{I,2} = 0$, and the proof is complete. $\square$

An immediate consequence of Theorem 2.4.8 is

Corollary 2.4.9. *Let* $\tilde{H} = \mathrm{Op}(\tau)$ *with* $\tau = \tau(y, \xi, \zeta)$ *and* $\tilde{P}(x) = \tilde{P} \in \mathfrak{S}(0, 1)$. *Then* $\sigma_I(H, P) = \sigma_I(\tilde{H}, \tilde{P})$.

Proof. Apply Theorem 2.4.8 to $H = \mathrm{Op}(\sigma)$ and $\tilde{H} = \mathrm{Op}(\tau)$. $\square$

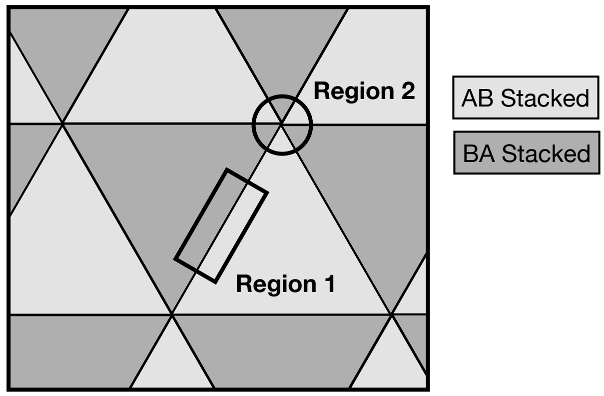

Figure 2.2: Triangular domains form in mechanically relaxed tBLG. We highlight two regions of interest for our analysis. Region 1 corresponds to an edge, resembling the setting in Sections 2.1–2.3. Region 2 is at a junction, where the theory from this subsection applies.

Observe that Corollary 2.4.9 reduces the junction conductivity to the simpler setting of a flat interface analyzed in Sections 2.1–2.3. The insulating materials are described by $\tau_\pm = \tau(\pm\infty, \xi, \zeta)$.

2.4.2 Applications

Twisted bilayer graphene (tBLG) is widely studied for its unique mechanical and electronic properties including the magic angle superconductivity [23, 18]. Upon gating, it acts as host of a network of topological interface channels, which can be seen experimentally and theoretically [74, 72, 24, 1]. tBLG is constructed by taking two periodic 2D sheets of graphene and stacking them with a relative twist, typically small. The atoms relax to minimize energy, forming large triangular regions of the energetically favorable AB and BA Bernal stacking [80, 24, 31]. It is relevant to note this asymmetric transport under gating is a separate phenomena from magic angle superconductivity. Indeed, the asymmetric transport phenomena only requires sufficiently small twist angles and vertical gating, i.e. by inducing a potential difference between the two layers, while superconductivity can only occur precisely at the magic twist angles. In this section, we make use of Figure 2.2 for discussion of the geometry. The interior of one of these triangles can be considered as approximately an infinite periodic material as the side of one of these triangles scales inversely proportional to the small twist angle [24].

Following the Bistritzer-MacDonald model [18], the junction Hamiltonian corresponding to Region 2 from Figure 2.2 is

$$\mathrm{Op}(\sigma) = H = \begin{pmatrix} \Omega I + D \cdot \sigma^{(\eta)} & \lambda U^*(x,y) \\ \lambda U(x,y) & -\Omega I + D \cdot \sigma^{(\eta)} \end{pmatrix}. \tag{2.4.11}$$

Here, λ and Ω are fixed real constants, $D \cdot \sigma^{(\eta)} := -i\partial_x \sigma_1 - i\eta\partial_y \sigma_2$ with $\eta \in \{-1, 1\}$, and $U(x,y) := \frac{1}{2}((1+\tilde{m}(x,y))A + (1-\tilde{m}(x,y))A^*)$. The function $\tilde{m} \in \mathcal{C}^\infty$ is positive in regions of AB stacking, negative in regions of BA stacking, and zero on the boundaries between regions. We assume that $\tilde{m} \in \{-1, 1\}$ away from these boundaries.

To construct such a function $\tilde{m}$ explicitly, define $f_\Theta : \mathbb{T} \to \mathbb{T}$ by $f_\Theta(\theta) = \sin(3\theta)$ and (as above) let $f \in \mathcal{C}^\infty(\mathbb{R}^2)$ such that $f(x,y) = rf_\Theta(\theta)$ for all $r \geq 1$, where (r, θ) are the polar coordinates corresponding to (x, y). For concreteness, take $f(x,y) := \chi(r) r f_\Theta(\theta)$, where $\chi \in \mathfrak{S}(0, 1; \varepsilon, 1)$ and $0 < \varepsilon < 1$. Since χ is smooth and vanishes near the origin, it is immediate that f is smooth.

Let $m \in \mathfrak{S}(-1, 1)$ be monotonically increasing with $m(0) = 0$, and define $\tilde{m}(x,y) := m(f(x,y))$. This definition is consistent with the above constraints, as $f_\Theta > 0$ if and only if $2k\pi/3 < \theta < (2k+1)\pi/3$ for some $k \in \{0, 1, 2\}$. Since m and all of its derivatives are bounded, it follows that $\sigma \in S^1_{1,0}$ with the right-hand side defined in Appendix B. Moreover, the structure of H (with $D \cdot \sigma^{(\eta)}$ on the diagonal and no other derivatives) implies the existence of a constant $c > 0$ such that $|\sigma_{\min}(x, y, \xi, \zeta)| \geq c\langle \xi, \zeta \rangle - 1$, where $\sigma_{\min}$ is the smallest magnitude eigenvalue of σ. We see that when $f(x, y)$ is sufficiently large (resp.

small), $\sigma = \sigma_+$ (resp. $\sigma = \sigma_-$), where

$$\sigma_+ = \begin{pmatrix} \Omega I + \xi\sigma_1 + \eta\zeta\sigma_2 & \lambda A^* \\ \lambda A & -\Omega I + \xi\sigma_1 + \eta\zeta\sigma_2 \end{pmatrix}$$

and

$$\sigma_- = \begin{pmatrix} \Omega I + \xi\sigma_1 + \eta\zeta\sigma_2 & \lambda A \\ \lambda A^* & -\Omega I + \xi\sigma_1 + \eta\zeta\sigma_2 \end{pmatrix}.$$

By [13, Appendix A], there exists $E > 0$ such that $\sigma_\pm$ (equivalently $H_\pm := \mathrm{Op}(\sigma_\pm)$) has a spectral gap in the interval $(E_1, E_2) := (-E, E)$.

Thus we have shown that H given by (2.4.11) satisfies (H1'), meaning that Theorem 2.4.8 applies. For concreteness, define $g_\Theta : \mathbb{T} \to \mathbb{T}$ by $g_\Theta(\theta) = \cos(\theta) + \cos(\pi/6) = \cos(\theta) + \sqrt{3}/2$ (note that $g_\Theta < 0$ if and only if $5\pi/6 < \theta < 7\pi/6$) and take $g(x, y) = \chi(r) r g_\Theta(\theta)$. Due to the factor of χ in the definition of g, the level set $g^{-1}(0)$ is not a curve in the $xy-$plane. Still, there exists a smooth function $(x_0, y_0) : \mathbb{R} \to \mathbb{R}^2$ whose range separates the $xy-$plane into two regions, R_+ and R_-, such that $g \geq 0$ in R_+ and $g \leq 0$ in R_-. More specifically, we can take

$$(x_0(t), y_0(t)) = \begin{cases} (\frac{\sqrt{3}}{2}t, \frac{1}{2}t), & t \leq -1 \\ (-\frac{\sqrt{3}}{2}t, \frac{1}{2}t), & t \geq 1 \end{cases}$$

and smoothly connect (x_0, y_0) for $|t| < 1$ so that $g(x_0(t), y_0(t)) = 0$ for all $t \in \mathbb{R}$. It follows that $\tau(t, \xi, \zeta) = \sigma_\pm(\xi, \zeta)$ whenever $\pm t > 0$ is sufficiently large, where τ is defined in terms of (x_0, y_0) by (2.4.5). By [13, Theorem 2.1], this means

$$2\pi\sigma_I(H, P, \varphi) = -2\eta\ \mathrm{sgn}(\Omega).$$

If $P_j = \chi_p(g_j(x,y))$ for $j \in \{0,1,2\}$ with the g_j appropriately chosen to satisfy the growth condition for $\langle f, g\rangle$, then $\sigma_I(H, \sum_j P_j, \varphi) = \sum_j \sigma_I(H, P_j, \varphi)$. Thus if $g_j(x,y) = \chi(r) r g_{j_\Theta}(\theta)$ with $g_{j_\Theta} = \cos(\theta - 2\pi j/3) + \cos(\pi/6)$, then the $2\pi/3-$rotational symmetry of the tBLG Hamiltonian implies that $\sigma_I(H, \sum_j P_j, \varphi) = 3\sigma_I(H, P_0, \varphi)$. That is, each term $\sigma_I(H, P_j, \varphi)$ in the sum over j sees the same transition from σ_- to σ_+. In words, the superposition of three appropriately chosen regularized indicator functions increases the conductivity by a factor of 3. This makes perfect sense, as the conductivity is now measured through three distinct regions (supp ∇P_j for $j = 0,1,2$), each of which contributes the same value of $-\eta\ \mathrm{sgn}(\Omega)/\pi$.

2×2 **Dirac Hamiltonian.** We conclude this section with an application of Theorem 2.4.8 to the operator

$$H = D_x\sigma_1 + D_y\sigma_2 + \tilde{m}(x,y)\sigma_3, \tag{2.4.12}$$

where $\tilde{m}(x,y) = m(f(x,y))$ for some $m \in \mathfrak{S}(-1,1)$, and

$$f(r,\theta) = \chi(r) r f_\Theta(\theta), \qquad \chi \in \mathfrak{S}(0,1;\varepsilon,1), \qquad f_\Theta(\theta) = \sin(k\theta)$$

for some $0 < \varepsilon < 1$ and $k \in \mathbb{N}_+$. Note that when $k = 1$, we recover the setting of a flat interface analyzed in detail in Sections 2.1–2.3, while $k = 3$ yields the same hexagonal structure on the right panel of Figure 2.1. As with the Bistritzer-MacDonald Hamiltonian (2.4.11), it is straightforward to verify that H defined by (2.4.12) satisfies (H1'), and thus the above theory applies. The bulk spectral gap in this case is $(E_1, E_2) = (-1, 1)$.

Take $P(x,y) = \chi_p(g(x,y))$ for $\chi_p \in \mathfrak{S}(0,1)$, where $g(x,y) = g(r,\theta) = \chi(r) r g_\Theta(\theta)$ and $g_\Theta(\theta) = \cos(\theta - \theta_1) - \cos(\theta_0)$, for some $0 < \theta_0 < \pi$ and $-\frac{\pi}{k} < \theta_1 < \frac{\pi}{k}$ satisfying

$$\theta_+ \notin \Theta_k, \quad 2\pi - \theta_+ \notin \Theta_k, \quad \Theta_k = \Big\{\frac{j}{k\pi} : j \in \mathbb{Z}\Big\}, \quad \theta_+ := \theta_0 + \theta_1.$$

This way, the zeros of g_Θ and f_Θ are disjoint. Indeed, $g_\Theta(\theta) = 0$ if and only if $\cos(\theta - \theta_1) =$

$\cos(\theta_0)$, which occurs exactly when $\{\theta + 2\pi j : j \in \mathbb{Z}\} \cap \{\theta_+, 2\pi - \theta_+\} \neq \emptyset$. It follows that $\tau(t, \xi, \zeta) = \xi\sigma_1 + \zeta\sigma_2 + \mu(t)\sigma_3$ for some $\mu \in \cup_{\varepsilon_1,\varepsilon_2 \in \{-1,1\}} \mathfrak{S}(\varepsilon_1, \varepsilon_2)$, where the ε_j are determined by θ_0 and θ_1. We have reduced the problem to computing the interface conductivity for the translation-invariant 2×2 Dirac system, and hence $2\pi\sigma_I = \frac{1}{2}(\varepsilon_1 - \varepsilon_2)$ by Section 2.3. For the case $(k, \theta_1) = (3, 0)$ which is analyzed numerically in the following section, we have

$$2\pi\sigma_I = \begin{cases} -1, & 0 < \theta_0 < \pi/3 \\ 1, & \pi/3 < \theta_0 < 2\pi/3 \\ -1, & 2\pi/3 < \theta_0 < \pi \end{cases} .$$

If g from Figure 2.1 were to have the above form, then $\theta_1 = 0$ and θ_0 would be the angle between [the line making up the top of the level curve $\{g = 0\}$] and [the positive $x-$axis]. So $\pi/2 < \theta_0 < \pi$ and $2\pi/3 < \theta_0 < \pi$ for the left and right panels, respectively.

CHAPTER 3

MAGNETIC DIRAC EQUATIONS

In this section, we derive a quantized conductivity at the interface of two (distinct) sheets of graphene (or other similar materials). As we will see below, the Hamiltonians considered here have symbols that are unbounded in the spatial coordinates (x, y) and not elliptic. As a result, none of the theory from Section 2 applies directly.

In the absence of external electric and magnetic fields, the edge state dynamics is governed by a two-dimensional Schrödinger Hamiltonian whose coefficients obey the appropriate honeycomb symmetry away from the interface. It was shown in [8, 36, 44] that at low energies, this Hamiltonian is well approximated by the following Dirac operator,

$$H_D = D_x\sigma_1 + D_y\sigma_2 + m(x)\sigma_3; \qquad D_\alpha := -i\partial_\alpha, \quad m \in \mathfrak{S}(m_-, m_+), \quad 0 \neq m_\pm \in \mathbb{R}.$$

Here, $\mathfrak{S}(a, b) := \cup_{\alpha<\beta}\mathfrak{S}(a, b; \alpha, \beta)$ with $\mathfrak{S}(a, b; \alpha, \beta)$ the set of smooth functions $f : \mathbb{R} \to \mathbb{R}$ such that $f(\lambda) = a$ (resp. $f(\lambda) = b$) whenever $\lambda \leq \alpha$ (resp. $\lambda \geq \beta$), and the Pauli matrices are given by

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

Observe that the interface material described by H_D is made up of two insulators (given by $H_\pm := D_x\sigma_1 + D_y\sigma_2 + m_\pm\sigma_3$) that are glued together along a one-dimensional interface, say $\{m(x) = 0\}$. The *mass term* m models the transition from one insulator to the other. Although $H_\pm$ has a spectral gap in the interval $(-|m_\pm|, |m_\pm|)$, the interface material is a conductor whenever m_+ and m_- have opposite sign. In this case H_D no longer has a spectral gap, and the energies in the interval $(-m_0, m_0)$ with $m_0 := \min\{|m_-|, |m_+|\}$ correspond to propagating edge modes as described above. As before, the asymmetric transport associated with this model is quantified by the following interface conductivity,

$$\sigma_I(H) := \operatorname{Tr} i[H,P]\varphi'(H). \tag{3.0.1}$$

Here, $P(y) = P \in \mathfrak{S}(0,1)$ and $\varphi \in \mathfrak{S}(0,1;-m_0,m_0)$. Explicit formulas for σ_I (that apply to H_D among other models) are derived in [10, 11]. In [7] it was shown that $2\pi\sigma_I(H_D) = \mathrm{SF}(H_D;\alpha) = \frac{1}{2}\operatorname{sgn}(m_+ - m_-)$, where $\mathrm{SF}(H_D;\alpha)$ is the *spectral flow of H_D through α* (more on this below) and $\alpha \in (-m_0,m_0)$. Observe that the quantity $\operatorname{sgn}(m_- - m_+)$ is independent of α, P and φ, and is robust with respect to changes in m.

The goal of this paper is to extend the above results for H_D to Dirac operators with electric and magnetic fields; we will explicitly calculate the interface conductivity by relating it to a spectral flow, and prove its stability in the presence of perturbations. The electromagnetic Dirac operators are given by

$$H = D_x\sigma_1 + (D_y - A_2(x))\sigma_2 + m(x)\sigma_3 + V(x)\sigma_0, \tag{3.0.2}$$

where $A_2(x) = xB(x)$ and

$$B \in \mathfrak{S}(B_-,B_+), \qquad m \in \mathfrak{S}(m_-,m_+), \qquad V \in \mathfrak{S}(V_-,V_+) \tag{3.0.3}$$

for some constants $B_\pm, m_\pm, V_\pm \in \mathbb{R}$ with $B_\pm \neq 0$. Here, σ_0 is the 2×2 identity matrix. The vector-valued function $A = (0, A_2)$ is the magnetic potential (in the Landau gauge), with $(B + xB')\hat{z} = \nabla \times A$ the magnetic field. The function V represents the electric potential. See [82, Section 4.2] for a derivation of these models.

We see that the Hamiltonian (3.0.2) implements three *domain walls* given by (3.0.3). The magnetic domain wall B gives rise to the unbounded term $A_2(x)$, while the functions m and V are necessarily bounded. We have already discussed the domain wall in m as a mechanism for transport. To motivate the domain wall in B, we provide an illustrative example.

Consider a two-dimensional electron gas confined to the right-half plane and subject to a constant (and strong) orthogonal magnetic field. Away from the edge $\{x = 0\}$ each electron will move in a (small) circular path, meaning the gas is insulating in its bulk. However the presence of the edge causes nearby electrons to propagate, giving rise to a current along the boundary. The same can be said of a (no longer confined) two-dimensional electron gas subject to an orthogonal magnetic field that changes signs across the $y-$axis.

The domain wall in V gives rise to an electric field $E = -\nabla V$ perpendicular to the interface that vanishes whenever $|x|$ is sufficiently large. Note that if the mass term were to grow linearly at infinity, the interface conductivity would no longer depend on the magnetic field [11].

The spectral properties of H are acquired from the following *bulk Hamiltonians*,

$$H_\pm = D_x\sigma_1 + (D_y - xB_\pm)\sigma_2 + m_\pm\sigma_3 + V_\pm\sigma_0,$$

which model the two insulating materials that are glued together to form the conductor with Hamiltonian H. Since H and $H_\pm$ are translation-invariant in y, we can define their Fourier transforms by

$$\hat{H}(\zeta) = D_x\sigma_1 + (\zeta - A_2(x))\sigma_2 + m(x)\sigma_3 + V(x)\sigma_0,$$
$$\hat{H}_\pm(\zeta) = D_x\sigma_1 + (\zeta - xB_\pm)\sigma_2 + m_\pm\sigma_3 + V_\pm\sigma_0$$

for $\zeta \in \mathbb{R}$. It is known that each operator $\mathcal{O} \in \{H, H_+, H_-, \hat{H}(\zeta), \hat{H}_+(\zeta), \hat{H}_-(\zeta)\}$ is self-adjoint with domain of definition $\mathcal{D}(\mathcal{O}) = (i - \mathcal{O})^{-1}\mathcal{H}$; see e.g. [11, 20, 82]. Here, $\mathcal{H} := L^2(\mathbb{R}^d) \otimes \mathbb{C}^2$, where $d = 2$ for H and $H_\pm$, and $d = 1$ for $\hat{H}$ and $\hat{H}_\pm$. Note that for a similar edge model, it was shown that the domain of definition of the Hamiltonian depends on the strength of the magnetic field [29]. This suggests that $\mathcal{D}(\mathcal{O})$ likely depends on $B_\pm$, though we do not investigate this issue here.

Throughout this thesis, we denote the spectrum of an operator $\mathcal{O}$ by $\sigma(\mathcal{O})$ and the resolvent set of $\mathcal{O}$ by $\rho(\mathcal{O})$. Suppose temporarily that $V_\pm = 0$, as these constants contribute merely a uniform shift to the spectrum of $H_\pm$. Then $\hat{H}^2_\pm(\zeta) = D_x^2 + (\zeta - xB_\pm)^2 + m_\pm^2 - B_\pm\sigma_3$ is block diagonal, meaning that up to shifts by $m_\pm^2 - B_\pm$ and $m_\pm^2 + B_\pm$, the spectra of $\hat{H}^2_\pm(\zeta)$ and $L_\pm(\zeta) := D_x^2 + (\zeta - xB_\pm)^2$ are the same. But $L_\pm(\zeta)$ is the Hamiltonian for the quantum harmonic oscillator (up to rescaling) and has spectrum consisting entirely of simple eigenvalues and given by $\sigma(L_\pm(\zeta)) = \{(2k+1)B : k \in \mathbb{N}\}$. The elements of $\sigma(L_\pm(\zeta))$ are known as "Landau levels." Since $\sigma(L_\pm(\zeta))$ (and hence $\sigma(\hat{H}_\pm(\zeta))$) is independent of ζ, it follows that $\sigma(H_\pm)$ is made up of a countable collection of points (all corresponding to essential spectrum now) going to infinity in absolute value; see Lemma 3.1.2. The domain wall in B can cause spectral gaps between Landau levels to close, with eigenvalues of $\hat{H}^2(\zeta)$ potentially going to infinity as $\zeta \to \pm\infty$; see Lemma 3.1.7.

When spectral branches of $\hat{H}(\zeta)$ do not go to infinity, they converge to elements of $\sigma(H_\pm)$ as shown by Lemma 3.1.6. Each branch converges both as $\zeta \to \infty$ and $\zeta \to -\infty$ in the case that B_+ and B_- have the same sign. When $B_- < 0 < B_+$ (resp. $B_+ < 0 < B_-$), the branches converge only as $\zeta \to \infty$ (resp. $\zeta \to -\infty$). Hence no matter the signs of B_+ and B_-, the branches of spectrum do not go to infinity as $|\zeta| \to \infty$. This means H lacks the *ellipticity* that is assumed by (H1) and in [10, 11, 37]. Indeed, the term $(D_y - A_2(x))\sigma_2$ has (Weyl) symbol $(\zeta - A_2(x))\sigma_2$, which can remain small even when $|\zeta|$ and $|x|$ are large.

Below is a brief summary of this section. We first define the spectral flow, and in doing so give an outline of Section 3.1. We refer to [66] for a more generally applicable definition. The set $\{\hat{H}(\zeta) : \zeta \in \mathbb{R}\}$ is a one-parameter family of self-adjoint operators, with $\hat{H}(\zeta)$ holomorphic in $\zeta \in \mathbb{C}$ (see [58, Chapter VII.1.1] for a precise definition of holomorphic operators). We will show with Lemmas 3.1.3 and 3.1.4 that the spectrum of $\hat{H}(\zeta)$ consists entirely of simple eigenvalues $\{\mu_j(\zeta)\}_{j\in\mathbb{Z}}$, where each *branch* $\mu_j : \mathbb{R} \to \mathbb{R}$ is analytic. Let

$$\mathcal{R} := \rho(H_+) \cap \rho(H_-) \cap \mathbb{R} \tag{3.0.4}$$

denote the bulk band gaps. It turns out that for any energy level $\alpha \in \mathcal{R}$, there exists $\zeta_\alpha > 0$ such that no branches attain the value α when $|\zeta| > \zeta_\alpha$ (Lemmas 3.1.6 and 3.1.7). Moreover, the number of branches to ever attain the value α is finite (Lemma 3.1.8).

This means we can define the *spectral flow of H through α* to be the signed number of crossings of branches through α:

$$\mathrm{SF}(H;\alpha) := N_\uparrow - N_\downarrow, \tag{3.0.5}$$

where $N_\uparrow$ (resp. $N_\downarrow$) is the number of branches that are less than α when $\zeta < -\zeta_\alpha$ and greater than α when $\zeta > \zeta_\alpha$ (resp. greater than α when $\zeta < -\zeta_\alpha$ and less than α when $\zeta > \zeta_\alpha$). With Theorem 3.1.1 we compute the spectral flow using the max-min principle [71, 81] and perturbation theory [58].

In Section 3.2, we relate the interface conductivity in (3.0.1) to the spectral flow in (3.0.5) (Theorem 3.2.5) and prove its stability under a large class of perturbations (Theorems 3.2.9–3.2.12). The stability results are proved using pseudo-differential calculus as in Section 2 and [10, 11, 37]. But since H is not elliptic, much of the pseudo-differential operator theory in this existing literature does not apply directly. Still, we are able to use Beals's criterion [34, Proposition 8.3] and specific properties of H (as a first-order differential operator with the spectrum of $H_\pm$ known) to obtain the necessary decay properties; see Lemmas 3.2.2 and 3.2.3. Similar stability results for (also non-elliptic) magnetic Schrödinger operators can be found in [28, 35].

3.1 Spectral analysis

In this section we calculate the spectral flow $\mathrm{SF}(H;\alpha)$ for $\alpha \in \mathcal{R}$, i.e. an energy level in a spectral gap for both bulk Hamiltonians. This involves analyzing the limiting behavior of the branches of spectrum $\mu_j(\zeta)$ of $\hat{H}(\zeta)$ as $|\zeta| \to \infty$. The multisets $S_\pm := \{\lim_{\zeta\to\pm\infty} \mu_j(\zeta)\}_{j\in\mathbb{Z}}$ are determined using a standard max-min argument. Perturbation theory is then used to match elements in S_+ with those in S_- to determine the quantities $\lim_{\zeta\to\pm\infty} \mu_j(\zeta)$ for every j. We now state the main result, which can be interpreted as a bulk-interface correspondence. We recall that $B_\pm \neq 0$ throughout this paper.

Theorem 3.1.1. *Fix $\alpha \in \mathcal{R}$. Then $SF(H;\alpha) = I(H_-;\alpha) - I(H_+;\alpha)$, where*

$$I(H_\pm;\alpha) = \operatorname{sgn}(B_\pm)\operatorname{sgn}(\alpha - V_\pm - m_\pm \operatorname{sgn}(B_\pm))\Big(N(H_\pm;\alpha) + \frac{1}{2}\Big) \tag{3.1.1}$$

and

$$N(H_\pm;\alpha) = \begin{cases} 0; & |\alpha - V_\pm| < \sqrt{2|B_\pm| + m_\pm^2}, \\ k; & \sqrt{2k|B_\pm| + m_\pm^2} < |\alpha - V_\pm| < \sqrt{2(k+1)|B_\pm| + m_\pm^2}, \quad k \in \mathbb{N}_+. \end{cases} \tag{3.1.2}$$

Note that $N(H_\pm;\alpha)$ counts the ($\zeta-$independent) number of eigenvalues of $\hat{H}_\pm(\zeta) - V_\pm$ in the interval $(|m_\pm|, |\alpha - V_\pm|)$. The above values of α for which $\mathrm{SF}(\alpha)$ is not defined are precisely the elements of $\sigma(H_+) \cup \sigma(H_-)$. Although the above expresses the (integer-valued) spectral flow as a difference of two bulk quantities, it is unclear whether each bulk quantity may be interpreted as an invariant as in [6, 16].

We refer to Figures 3.1–3.3 for an illustration of the branches of spectrum of H, under various choices of the parameters $B_\pm, m_\pm$ and $V_\pm$. [1] For example, in the top right panel of

1. These figures were generated using a standard finite difference approximation of the Hamiltonian with

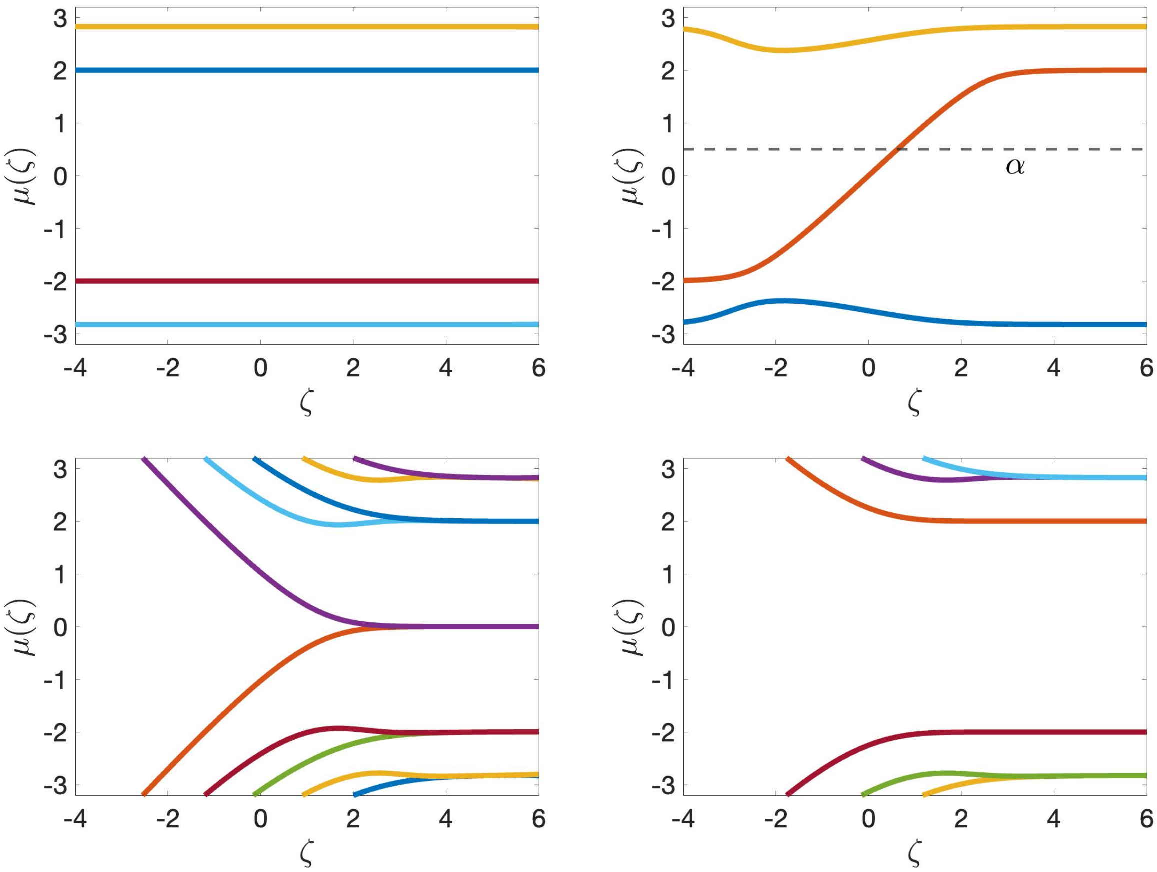

Figure 3.1: Plots of the lowest-magnitude eigenvalues of $\hat{H}(\zeta)$ as a function of ζ, for different combinations of domain walls in B and m. For all plots, $V \equiv 0$. The choices of parameters are $B \equiv 2$ and $m \equiv 2$ (top left); $B \equiv 2$ and $m_+ = 2 = -m_-$ (top right); $B_+ = 2 = -B_-$ and $m \equiv 0$ (bottom left); $B_+ = 2 = -B_-$ and $m \equiv 2$ (bottom right). As $\zeta \to +\infty$, these eigenvalues converge to the elements of $\sigma(\hat{H}_+(\zeta)) \cup \sigma(\hat{H}_+(\zeta))$ as predicted by the theory; see Lemma 3.1.7. The top left panel illustrates the spectrum of a bulk Hamiltonian; see Lemma 3.1.2. As demonstrated by the top right plot, a transition in the sign of m generates a nonzero spectral flow for α near 0 (in this example, $\mathrm{SF}(H;\alpha) = 1$). Comparing the two bottom plots, we see how a constant nonzero m opens a gap at 0. Although it may look like the eigenvalues in the bottom plots are degenerate for large ζ, this is not the case (Lemma 3.1.3). They only have the same limit as $\zeta \to \infty$.

Figure 3.2 we see that $\mathrm{SF}(H;\alpha) = 1$ for all α near 0, while $\mathrm{SF}(H;\alpha) = -1$ for any α near 2.5.

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periodic boundary conditions. The periodic Hamiltonian also has spurious eigenvalues (corresponding to eigenfunctions that are localized near the boundary; see Section 4 for more details), which are not included in our plots.

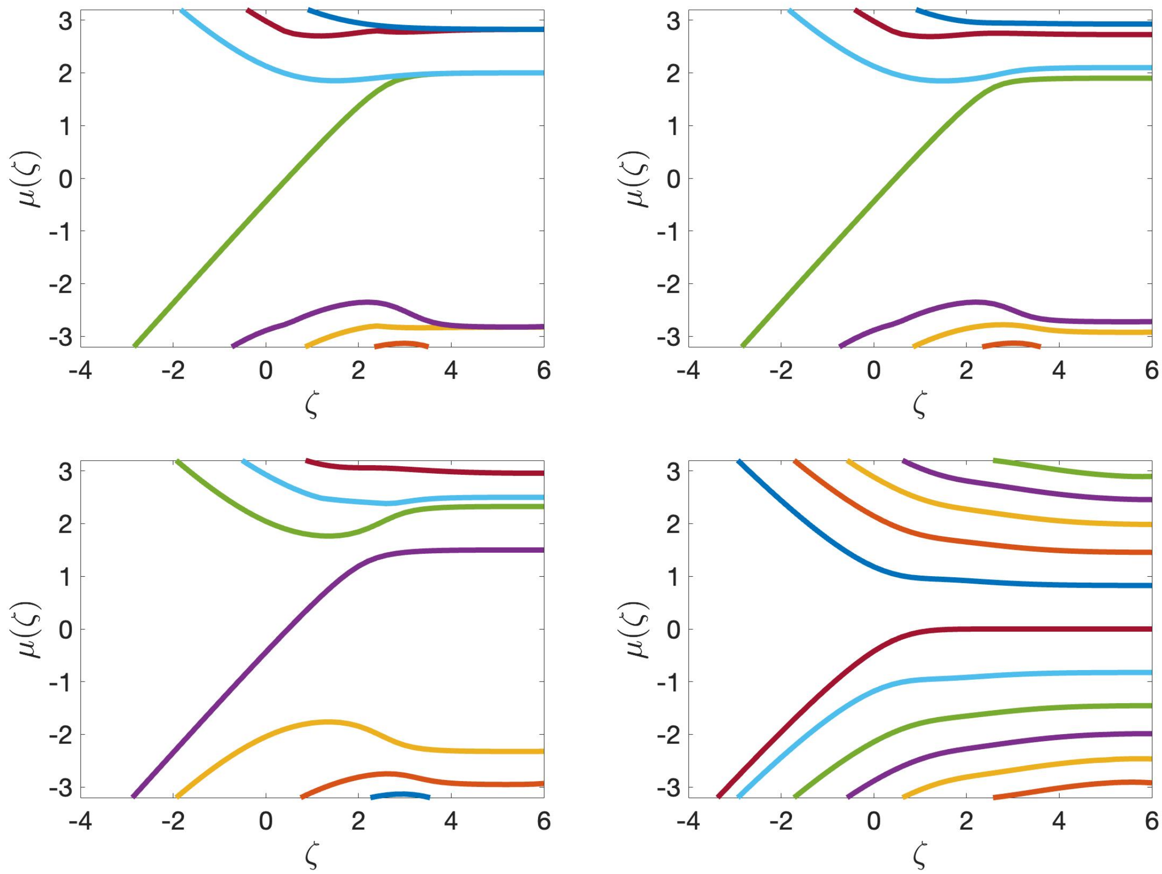

Figure 3.2: Effect of the electric potential V on the lowest-magnitude eigenvalues of $\hat{H}(\zeta)$. All plots have $B_+ = 2 = -B_-$ and $m_+ = 2 = -m_-$. The choices of electric potential are $V \equiv 0$ (top left); $V_+ = 0.1 = -V_-$ (top right); $V_+ = 0.5 = -V_-$ (bottom left); $V_+ = 2 = -V_-$ (bottom right). Notice that, as predicted by Lemma 3.1.2, a small domain wall in V opens a gap between pairs of branches for large ζ (top panels).

The rest of this section is devoted to proving Theorem 3.1.1 (and the statements we made before it). We begin by determining the spectrum of $\hat{H}_\pm(\zeta)$.

Lemma 3.1.2. *For any $\zeta \in \mathbb{R}$, the spectrum of $\hat{H}_\pm(\zeta)$ consists entirely of eigenvalues and*

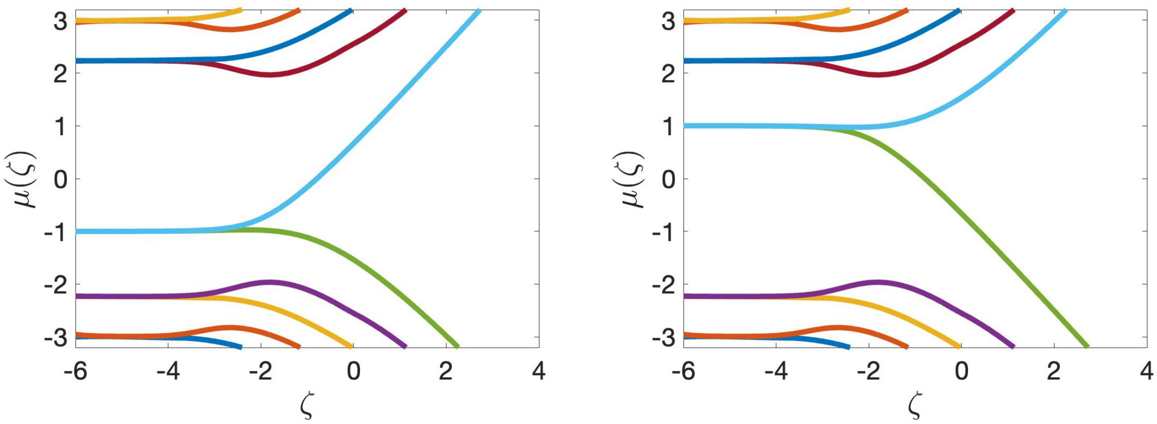

Figure 3.3: Effect of the signs of $B_\pm$ and $m_\pm$ on the lowest-magnitude eigenvalues of $\hat{H}(\zeta)$. Both plots have $-B_+ = 2 = B_-$ and $V \equiv 0$. The left panel corresponds to $m_+ = 1 = -m_-$ and the right to $-m_+ = 1 = m_-$. Since $B_+ < 0 < B_-$ (in contrast with Figures 3.1 and 3.2), the branches now converge to the elements of $\sigma(\hat{H}_+(\zeta)) \cup \sigma(\hat{H}_+(\zeta))$ as $\zeta \to -\infty$ while going to infinity as $\zeta \to +\infty$. By comparing the left and right panels, observe that the sign-flips in $m_\pm$ change the spectral flow only for $-1 < \alpha < 1$.

is given by

$$\sigma(\hat{H}_\pm(\zeta)) = \{\varepsilon\sqrt{2k|B_\pm| + m_\pm^2} + V_\pm : \varepsilon \in \{-1,1\}, k \in \mathbb{N}_+\} \bigcup \{m_\pm \operatorname{sgn}(B_\pm) + V_\pm\}. \tag{3.1.3}$$

Above, the subscripts $\pm$ (and one operation $\mp$) are understood to correspond to the operator $\hat{H}_\pm$ in question. Note that the spectrum of $\hat{H}_\pm(\zeta)$ is independent of ζ; thus the spectrum of $H_\pm$ is also given by (3.1.3), only now these values all belong to the *essential spectrum.*

Proof. Suppose for concreteness that $B_+ > 0$. Set $V_+ = 0$ without loss of generality, as this term only contributes a uniform shift of the spectrum. Any eigenpair μ and ψ of $\hat{H}_+(\zeta)$ must satisfy $\hat{H}_+^2(\zeta)\psi = \mu^2\psi$, with $\hat{H}_+^2(\zeta) = D_x^2 + (\zeta - B_+x)^2 + m_+^2 - B_+\sigma_3$. The eigenelements of $\hat{H}_+^2(\zeta)$ are well known. The eigenvalues are $\nu_k = 2k|B_+| + m_+^2$ for $k \in \mathbb{N}$. When $k \in \mathbb{N}_+$, ν_k has multiplicity 2 and the eigenfunctions are $\psi_{k,\uparrow} = (\phi_k, 0)$ and $\psi_{k,\downarrow} = (0, \phi_{k-1})$, where $\phi_k(x) = |B_+|^{-1/4}\tilde{\phi}_k(\sqrt{|B_+|}x - \zeta)$ with $\tilde{\phi}_k$ the Hermite functions.

We see that ν_0 has multiplicity one with eigenfunction $\psi_0 = (\phi_0, 0)$. We then verify that the eigenvalues of $\hat{H}_+(\zeta)$ are $\mu_{k,\varepsilon} = \varepsilon\sqrt{\nu_k}$ for $\varepsilon \in \{-1, 1\}$, $k \in \mathbb{N}_+$ and $\mu_0 = m_+$, with corresponding eigenfunctions $\psi_{k,\varepsilon} = c_{1,\varepsilon}\psi_{k,\uparrow} + c_{2,\varepsilon}\psi_{k,\downarrow}$ and ψ_0 for some $|c_{1,\varepsilon}|^2 + |c_{2,\varepsilon}|^2 = 1$. If instead $B_+ < 0$, we would instead have $\psi_{k,\uparrow} = (\phi_{k-1}, 0)$ and $\psi_{k,\downarrow} = (0, \phi_k)$. All elements of the spectrum would be the same as before with the exception of $\mu_0 = -m_+$ now. The eigenelements of $\hat{H}_-(\zeta)$ are calculated similarly. This completes the result. $\square$

The following two lemmas state important properties of the spectrum of $\hat{H}(\zeta)$, with $\zeta \in \mathbb{C}$ now. The extension to complex ζ will be necessary when we later apply the holomorphic perturbation theory from [58].

Lemma 3.1.3. *For any $\zeta \in \mathbb{C}$, the spectrum of $\hat{H}(\zeta)$ consists entirely of simple eigenvalues.*

Proof. Fix $\zeta_0 + i\zeta_1 := \zeta \in \mathbb{C}$. We know that $\hat{H}(\zeta_0)$ is self-adjoint [11, 20, 82], hence $|\Im\mu| \le |\zeta_1|$ for all $\mu \in \sigma(\hat{H}(\zeta))$. The Weyl symbol (see Appendix A.1 for the definition) of $\hat{H}(\zeta)$ grows linearly in $\langle x, \xi \rangle$, as demonstrated by (3.2.2) below. This implies that $(i(1 + |\zeta_1|) + \hat{H}(\zeta))^{-1}$ is compact (see e.g. [11, 20]), and hence $\sigma(\hat{H}(\zeta))$ consists entirely of eigenvalues. We now prove that each eigenvalue has multiplicity one. Suppose ψ and ϕ are eigenfunctions of $\hat{H}$ corresponding to eigenvalue μ. This means

$$
\begin{aligned}
-i\psi_2' - i(\zeta - A_2)\psi_2 + (V + m)\psi_1 &= \mu\psi_1 \\
-i\psi_1' + i(\zeta - A_2)\psi_1 + (V - m)\psi_2 &= \mu\psi_2,
\end{aligned}
$$

with the same equations holding also with ψ replaced by ϕ. It follows that

$$
\psi_1\phi_2' + \psi_1'\phi_2 = i(\mu - m - V)\psi_1\phi_1 + i(\mu + m - V)\psi_2\phi_2 = \psi_2\phi_1' + \psi_2'\phi_1,
$$

so that

$$\partial_x(\psi_1\phi_2 - \psi_2\phi_1) = \psi_1\phi_2' + \psi_1'\phi_2 - (\psi_2\phi_1' + \psi_2'\phi_1) = 0.$$

Since ψ, ϕ, ψ', ϕ' all go to zero as $|x| \to \infty$, we have shown that $\psi_1\phi_2 - \psi_2\phi_1 \equiv 0$. Thus for every $x \in \mathbb{R}$, the vectors $(\psi_1(x), \psi_2(x))$ and $(\phi_1(x), \phi_2(x))$ are linearly dependent. Normalize the eigenfunctions so that $\psi(x_0) = \phi(x_0)$ for some $x_0 \in \mathbb{R}$ (this can be done because ψ and ϕ are continuous, hence there must exist a point at which both functions are zero or both functions are nonzero). Letting $\nu := \psi - \phi$, we see that

$$\nu'(x) = F(x)\nu(x), \quad x \in \mathbb{R}; \qquad\qquad \nu(x_0) = 0,$$

for some $F \in \mathcal{C}^\infty(\mathbb{R}; \mathbb{C}^{2\times 2})$. By regularity of F, the standard uniqueness result for first-order ODE implies that $\nu \equiv 0$. This completes the result. □

Lemma 3.1.4. *There exists a countable collection of holomorphic functions,* $\{\mu_j\}_{j\in\mathbb{Z}} \subset \mathcal{C}^\omega(\mathbb{C})$*, such that for each* $\zeta \in \mathbb{C}$*,* $\sigma(\hat{H}(\zeta)) = \{\mu_j(\zeta) : j \in \mathbb{Z}\}$*. The corresponding eigenprojections are also holomorphic in* $\zeta \in \mathbb{C}$*. Finally, the restriction of each* μ_j *to the real axis defines a real-analytic function.*

Here, $\mathcal{C}^\omega(\mathbb{C})$ denotes the set of holomorphic functions on $\mathbb{C}$. We refer to [58, Chapter VII.1.1] for the precise definition of an operator-valued holomorphic function.

Proof. Note that $\hat{H}(\zeta)$ is holomorphic in $\zeta \in \mathbb{C}$, thus Lemma 3.1.3 and [58, Theorems VII.1.7 and VII.1.8] imply that the eigenvalues and eigenprojections of $\hat{H}(\zeta)$ are also holomorphic in $\zeta \in \mathbb{C}$. That μ_j maps $\mathbb{R}$ to itself follows directly from the self-adjointness of $\hat{H}(\zeta)$ when $\zeta \in \mathbb{R}$. □

Henceforth (unless otherwise specified) it is assumed that $\zeta \in \mathbb{R}$. We now show that bounded perturbations of $\hat{H}$ cannot change the μ_j by too much.

Lemma 3.1.5. *Let $m_j \in \mathfrak{S}(m_{j,-}, m_{j,+})$ and $V_j \in \mathfrak{S}(V_{j,-}, V_{j,+})$ for $j \in \{1,2\}$, where the $m_{j,\pm}$ and $V_{j,\pm}$ are real numbers. For $\zeta \in \mathbb{R}$ and $\lambda \in [0,1]$, set*

$$\begin{aligned}\hat{H}(\zeta,\lambda) = D_x\sigma_1 + (\zeta - A_2(x))\sigma_2 + m_1(x)\sigma_3 + V_1(x)\sigma_0 \\ + \lambda((m_2(x) - m_1(x))\sigma_3 + (V_2(x) - V_1(x))\sigma_0).\end{aligned}$$

Let $\{\mu_j(\zeta,\lambda)\}_{j\in\mathbb{Z}}$ denote the eigenvalues of $\hat{H}(\zeta,\lambda)$. Then the μ_j can be chosen real-analytic in $(\zeta,\lambda) \in \mathbb{R} \times [0,1]$ and

$$|\partial_\lambda \mu_j(\zeta,\lambda)| \leq \|m_2 - m_1\|_\infty + \|V_2 - V_1\|_\infty .$$

Proof. Since m and V were arbitrary switch functions, it follows from Lemma 3.1.3 and [58, Theorems VII.1.7 and VII.1.8] as before that the eigenvalues and eigenprojections of $\hat{H}(\zeta,\lambda)$ are holomorphic in $(\zeta,\lambda) \in \mathbb{C}^2$. Since the eigenvalues are real whenever ζ and λ are real, we have proved the first part of the lemma. Letting $\mu(\zeta,\lambda)$ denote such an eigenvalue with $\Pi_{\zeta,\lambda} = \psi_{\zeta,\lambda}\psi^*_{\zeta,\lambda}$ the projection onto the corresponding (one-dimensional) eigenspace, we have

$$\hat{H}(\zeta,\lambda)\psi_{\zeta,\lambda} = \mu(\zeta,\lambda)\psi_{\zeta,\lambda}.$$

Now fix $\zeta \in \mathbb{R}$ and $\lambda \in [0,1]$, and let $h > 0$. Evaluating the difference of the above between λ and $\lambda + h$ yields

$$\begin{aligned}&(\hat{H}(\zeta,\lambda+h) - \hat{H}(\zeta,\lambda))\psi_{\zeta,\lambda+h} + \hat{H}(\zeta,\lambda)(\psi_{\zeta,\lambda+h} - \psi_{\zeta,\lambda}) \\ &\quad = \hat{H}(\zeta,\lambda+h)\psi_{\zeta,\lambda+h} - \hat{H}(\zeta,\lambda)\psi_{\zeta,\lambda} = \mu(\zeta,\lambda+h)\psi_{\zeta,\lambda+h} - \mu(\zeta,\lambda)\psi_{\zeta,\lambda} \\ &\quad = (\mu(\zeta,\lambda+h) - \mu(\zeta,\lambda))\psi_{\zeta,\lambda+h} + \mu(\zeta,\lambda)(\psi_{\zeta,\lambda+h} - \psi_{\zeta,\lambda}).\end{aligned}$$

Multiplying both sides by $\bar{\psi}_{\zeta,\lambda}$ and taking inner products, we obtain

$$(\psi_{\zeta,\lambda}, (\hat{H}(\zeta, \lambda + h) - \hat{H}(\zeta, \lambda))\psi_{\zeta,\lambda+h}) = (\mu(\zeta, \lambda + h) - \mu(\zeta, \lambda))(\psi_{\zeta,\lambda}, \psi_{\zeta,\lambda+h}).$$

Using that $\hat{H}(\zeta, \lambda + h) - \hat{H}(\zeta, \lambda) = h((m_2(x) - m_1(x))\sigma_3 + (V_2(x) - V_1(x))\sigma_0)$, we divide both sides by h to get

$$\begin{aligned}(\psi_{\zeta,\lambda}, ((m_2(x) - m_1(x))\sigma_3 + (V_2(x) - V_1(x))\sigma_0)\psi_{\zeta,\lambda+h})& \\ = h^{-1}(\mu(\zeta, \lambda + h) - \mu(\zeta, \lambda))(\psi_{\zeta,\lambda}, \psi_{\zeta,\lambda+h}).&\end{aligned} \tag{3.1.4}$$

Since $\Pi_{\zeta,\lambda}$ is holomorphic in λ, the operator norm $\|\Pi_{\zeta,\lambda+h} - \Pi_{\zeta,\lambda}\|$ goes to zero as $h \to 0$. Hence

$$\|(\psi_{\zeta,\lambda+h}, \psi_{\zeta,\lambda})\psi_{\zeta,\lambda+h} - \psi_{\zeta,\lambda}\| \to 0,$$

meaning that $|(\psi_{\zeta,\lambda+h}, \psi_{\zeta,\lambda})| \to 1$. Taking the absolute value of (3.1.4) and sending $h \to 0$, we thus obtain

$$|\partial_\lambda \mu(\zeta, \lambda)| \leq \|m_2 - m_1\|_\infty + \|V_2 - V_1\|_\infty .$$

This completes the proof. □

Next we determine the multisets $\{\lim_{\zeta\to\pm\infty} \mu_j(\zeta)\}_{j\in\mathbb{Z}}$, which depend on the signs of B_+ and B_-. Given two sets A and B, we use the notation $A+B$ to denote the multiset formed by combining A and B. That is, $x \in A + B$ if and only if $x \in A \cup B$, where the multiplicity of x is 2 if $x \in A \cap B$ and 1 otherwise. Although each μ_j has multiplicity 1 (Lemma 3.1.3), it is possible that two distinct μ_j converge to the same value (as $\zeta \to \infty$ if $B_- < 0 < B_+$; as $\zeta \to -\infty$ if $B_+ < 0 < B_-$).

Lemma 3.1.6. *1. Suppose $B_- < 0 < B_+$. Then for each $j \in \mathbb{Z}$, $\mu_{j,\infty} := \lim_{\zeta\to\infty} \mu_j(\zeta)$ exists and belongs to $\sigma(\hat{H}_+(\zeta)) \cup \sigma(\hat{H}_-(\zeta))$. For each $\nu \in \sigma(\hat{H}_+(\zeta)) + \sigma(\hat{H}_-(\zeta))$, there* *exists exactly one index $j \in \mathbb{Z}$ such that $\mu_{j,\infty} = \nu$.*

2. *Suppose $B_+ < 0 < B_-$. Then for each $j \in \mathbb{Z}$, $\mu_{j,-\infty} := \lim_{\zeta \to -\infty} \mu_j(\zeta)$ exists and belongs to $\sigma(\hat{H}_+(\zeta)) \cup \sigma(\hat{H}_-(\zeta))$. For each $\nu \in \sigma(\hat{H}_+(\zeta)) + \sigma(\hat{H}_-(\zeta))$, there exists exactly one index $j \in \mathbb{Z}$ such that $\mu_{j,-\infty} = \nu$.*

3. *Suppose $0 < B_+, B_-$. Then for each $j \in \mathbb{Z}$, $\mu_{j,\pm\infty} := \lim_{\zeta \to \pm\infty} \mu_j(\zeta)$ exists and belongs to $\sigma(\hat{H}_\pm(\zeta))$. For each $\nu \in \sigma(\hat{H}_\pm(\zeta))$, there exists exactly one index $j \in \mathbb{Z}$ such that $\mu_{j,\pm\infty} = \nu$.*

4. *Suppose $B_+, B_- < 0$. Then for each $j \in \mathbb{Z}$, $\mu_{j,\pm\infty} := \lim_{\zeta \to \pm\infty} \mu_j(\zeta)$ exists and belongs to $\sigma(\hat{H}_\mp(\zeta))$. For each $\nu \in \sigma(\hat{H}_\mp(\zeta))$, there exists exactly one index $j \in \mathbb{Z}$ such that $\mu_{j,\pm\infty} = \nu$.*

Proof. Suppose $B_- < 0 < B_+$. Let $\{\nu_{k,\pm} : k \in \mathbb{N}\}$ denote the full set of eigenvalues of $\hat{H}_\pm$. Applying the max-min principle (Theorem 4.1.5) to $\hat{H}^2(\zeta)$ (see [30, 88] and Section 4.1 for similar arguments), it follows that there is a bijection $\iota : \mathbb{Z} \to \mathbb{N} \times \{+,-\}$ such that for every $j \in \mathbb{Z}$, $\mu_j^2(\zeta) \to \nu_{\iota(j)}^2$ as $\zeta \to \infty$.

Now fix $j \in \mathbb{Z}$ and let $K_j := \{i \in \mathbb{Z} : \nu_{\iota(i)}^2 = \nu_{\iota(j)}^2\}$. (Lemma 3.1.2 implies that K_j can have at most four elements.) By Lemma 3.1.5, the quantities $\lim_{\zeta \to \infty} \mu_j^2(\zeta)$ are continuous in shifts of V. Thus there is a bijection $\iota_j : K_j \to \iota(K_j)$ such that for all $i \in K_j$ and α sufficiently small, $(\mu_i(\zeta) + \alpha)^2 \to (\nu_{\iota_j(i)} + \alpha)^2$ as $\zeta \to \infty$. Indeed, the previous paragraph applies also to $H + \alpha$, as $V \in \mathfrak{S}(V_-, V_+)$ was arbitrary. Hence $\lim_{\zeta \to \infty} \mu_i(\zeta) = \nu_{\iota_j(i)}$ for all $i \in K_j$, as desired.

The proofs for cases 2–4 are similar. $\square$

Lemma 3.1.7. 1. *Suppose $B_- < 0 < B_+$. For every $M > 0$, there exists $\zeta_0 \in \mathbb{R}$ such that $|\mu_j(\zeta)| > M$ for all $\zeta < \zeta_0$ and $j \in \mathbb{Z}$.*

2. *Suppose $B_+ < 0 < B_-$. For every $M > 0$, there exists $\zeta_0 \in \mathbb{R}$ such that $|\mu_j(\zeta)| > M$ for all $\zeta > \zeta_0$ and $j \in \mathbb{Z}$.*

By continuity of the μ_j, Lemma 3.1.7 implies that when $\pm B_- < 0 < \pm B_+$, each μ_j goes either to $+\infty$ or $-\infty$ as $\zeta \to \mp\infty$.

Proof. Suppose $B_- < 0 < B_+$. We see that

$$\begin{aligned}\hat{H}^2(\zeta) = D_x^2 + (\zeta - A_2(x))^2 + m^2(x) - A_2'(x)\sigma_3 - m'(x)\sigma_2 + V^2(x) \\ + 2V(x)(D_x\sigma_1 + (\zeta - A_2(x))\sigma_2 + m(x)\sigma_3) - iV'(x)\sigma_1,\end{aligned} \tag{3.1.5}$$

where σ_0 has been dropped from the notation. Since V is bounded, we know there exists a constant $C > 0$ such that

$$|(\psi, VD_x\sigma_1\psi)| \leq C \|\psi\| \|\psi'\|$$

for all $\psi \in \mathcal{H}^1$. Since $(\psi, D_x^2\psi) = \|\psi'\|^2$, it follows that the operator $D_x^2 + V(x)D_x\sigma_1$ is bounded from below. The function A_2 is also bounded from below, hence

$$\lim_{\zeta\to-\infty} \inf_{x\in\mathbb{R}} (\zeta - A_2(x))^2 = \infty.$$

Since m, V, m', V', A_2' are all bounded, we conclude that all eigenvalues of $\hat{H}^2(\zeta)$ go to infinity uniformly as $\zeta \to -\infty$. The proof for the case $B_+ < 0 < B_-$ is similar. This completes the result. □

We also need the following result, which ensures that the spectral flow is well defined.

Lemma 3.1.8. *For every $\alpha \in \mathcal{R}$, the set $\mathcal{T}_\alpha := \{j : \alpha \in \mathrm{Ran}(\mu_j)\}$ is finite.*

Above, $\mathrm{Ran}(\mu_j) := \{\mu_j(\zeta) : \zeta \in \mathbb{R}\}$ is the *range* (or image) of μ_j.

Proof. Fix $\alpha \in \mathcal{R}$. The previous lemmas imply the existence of $\bar{\zeta} > 0$ such that $\mu_j(\zeta) \neq \alpha$ for all $j \in \mathbb{Z}$ and $|\zeta| > \bar{\zeta}$. For $\zeta \in \mathbb{R}$ and $\beta > 0$, let $N(\zeta, \beta) := |\{j : \mu_j^2(\zeta) < \beta\}|$. Suppose by contradiction that $\mathcal{T}_\alpha$ is infinite. Then there exists a sequence $(\zeta_k) \subset [-\bar{\zeta}, \bar{\zeta}]$ and a number $\zeta_* \in [-\bar{\zeta}, \bar{\zeta}]$ such that $\zeta_k \to \zeta_*$ and $N(\zeta_k, \alpha^2) \to \infty$ as $k \to \infty$. But Lemma 3.1.3 implies that $N(\zeta_*, \alpha^2 + 1) < \infty$, hence there exist $i, j \in \mathbb{Z}$ such that $\mu_i(\zeta_*) \leq -\sqrt{\alpha^2 + 1}$ and $\mu_j(\zeta_*) \geq \sqrt{\alpha^2 + 1}$. Lemma 3.1.3 and the fact that $N(\zeta_k, \alpha^2) \to \infty$ imply that for all k sufficiently large, there exists $\ell \in \{i, j\}$ such that $\mu_\ell^2(\zeta_k) < \alpha^2$. Thus either μ_i or μ_j is not continuous at ζ_*, which contradicts Lemma 3.1.4. □

To compute the spectral flow in (3.0.5), it remains to determine the sign of $\mu_j(\zeta)$ as $\zeta \to -\infty$. We will do this first by imposing additional constraints on $\hat{H}$.

Lemma 3.1.9. *Fix $\zeta \in \mathbb{R}$, let $m_0 \in \mathbb{R}$ such that $m_0^2 > \|A_2'\|_\infty$, and define*

$$\hat{H}_0(\zeta) := D_x \sigma_1 + (\zeta - A_2(x))\sigma_2 + m_0 \sigma_3.$$

Then $\hat{H}_0(\zeta)$ has a spectral gap in the interval $(-\Delta, \Delta)$, with $\Delta := \sqrt{m_0^2 - \|A_2'\|_\infty}$.

The above implies that for $\hat{H}_0$, if $B_- < 0 < B_+$, every branch converging to a positive (resp. negative) value as $\zeta \to \infty$ goes to $+\infty$ (resp. $-\infty$) as $\zeta \to -\infty$.

Proof. Observe that $\hat{H}_0^2(\zeta) := D_x^2 + (\zeta - A_2(x))^2 + m_0^2 - A_2'(x)\sigma_3$, and the result easily follows. □

We are now ready to complete the proof of Theorem 3.1.1. The idea is to treat $\hat{H}$ as a perturbation of $\hat{H}_0$. For $\zeta \in \mathbb{R}$ and $(\lambda_1, \lambda_2) \in [0, 1]^2$, define

$$\hat{H}(\zeta; \lambda_1, \lambda_2) := D_x \sigma_1 + (\zeta - A_2(x))\sigma_2 + m_0 \sigma_3 + \lambda_1 (m(x) - m_0)\sigma_3 + \lambda_2 V(x)\sigma_0,$$

and let $\{\mu_j(\zeta; \lambda_1, \lambda_2)\}_{j \in \mathbb{Z}}$ denote the eigenvalues of $\hat{H}(\zeta; \lambda_1, \lambda_2)$. We use the shorthand $\lambda := (\lambda_1, \lambda_2)$ and $\mu_{j, \pm\infty}(\lambda) := \lim_{\zeta \to \pm\infty} \mu_j(\zeta; \lambda)$. By Lemma 3.1.5, the $\mu_j(\zeta; \lambda)$ are real-analytic in $(\zeta; \lambda) \in \mathbb{R} \times [0, 1]^2$ with $\partial_{\lambda_i} \mu_j(\zeta; \lambda)$ bounded uniformly in $(\zeta; \lambda)$ for $i \in \{1, 2\}$.

This means the limits as $\zeta \to \pm\infty$ of the $\mu_j(\zeta;\lambda)$ depend continuously on λ. Recall that Lemmas 3.1.6, 3.1.7 and 3.1.9 give us a full description of the $\mu_j(\zeta;0,0)$.

When $B_- < 0 < B_+$, the $\mu_{j,\infty}(0,0)$ are known (and finite) and $\mu_{j,-\infty}(0,0) = \pm\infty$ if and only if $\pm\mu_{j,\infty}(0,0) > 0$. The uniform bounds on $\partial_{\lambda_i}\mu_j$ imply that $\mu_{j,-\infty}(\lambda) = \mu_{j,-\infty}(0,0)$ for all $\lambda \in [0,1]^2$. Combined with Lemma 3.1.3 and the fact that the multiset $\{\mu_{j,\infty}(1,1)\}_{j\in\mathbb{Z}}$ is known (Lemmas 3.1.2 and 3.1.6), this will allow us to obtain the limits as $\zeta \to \pm\infty$ of each $\mu_j(\zeta;1,1)$ via a smooth transition of λ from $(0,0)$ to $(1,1)$. We find it easiest to first fix $\lambda_2 = 0$ while smoothly varying λ_1 from 0 to 1; then fix $\lambda_1 = 1$ while smoothly varying λ_2 from 0 to 1. The case $B_+ < 0 < B_-$ is handled similarly.

When $0 < B_+, B_-$, Lemma 3.1.6 gives us the multisets $L_\pm := \{\mu_{j,\pm\infty}(\lambda)\}_{j\in\mathbb{Z}}$ for all $\lambda \in [0,1]^2$. The only thing left is to pair each element of L_- with an element of L_+ (i.e. for each $\mu_{j,-\infty}(\lambda) \in L_-$, determine $\mu_{j,+\infty}(\lambda)$). When $\lambda = (0,0)$, this pairing follows immediately from Lemma 3.1.9. That is (using a natural choice of indices),

$$\ldots, \quad \mu_{-1,\pm\infty}(0,0) = -\sqrt{2|B_\pm| + m_0^2}, \quad \mu_{0,\pm\infty}(0,0) = m_0, \\ \mu_{1,\pm\infty}(0,0) = \sqrt{2|B_\pm| + m_0^2}, \quad \ldots$$

Since $\mu_{i,\pm\infty}(\lambda) \neq \mu_{j,\pm\infty}(\lambda)$ whenever $i \neq j$, it is straightforward to obtain the limits of each μ_j for $\lambda = (1,1)$ (again by a smooth transition from $\lambda = (0,0)$ to $\lambda = (1,1)$). The case $B_+, B_- < 0$ is handled similarly.

Proof of Theorem 3.1.1. Take m_0 as in Lemma 3.1.9. As in Lemma 3.1.5 the eigenvalues and eigenprojections of $\hat{H}(\zeta;\lambda)$ are holomorphic in $(\zeta;\lambda)$. It then follows from Lemma 3.1.5 that

$$|\partial_{\lambda_1}\mu(\zeta,\lambda)| \le \|m - m_0\|_\infty, \qquad |\partial_{\lambda_2}\mu(\zeta,\lambda)| \le \|V\|_\infty \tag{3.1.6}$$

for all eigenvalues $\mu(\zeta;\lambda)$ of $\hat{H}(\zeta;\lambda)$. Define

$$\hat{H}_{\pm}(\zeta;\lambda_1,\lambda_2) := D_x\sigma_1 + (\zeta - xB_{\pm})\sigma_2 + m_0\sigma_3 + \lambda_1(m_{\pm} - m_0)\sigma_3 + \lambda_2 V_{\pm}\sigma_0.$$

Lemma 3.1.2 states that the spectrum of $\hat{H}_{\pm}(\zeta;0,0)$ consists entirely of eigenvalues and is given by

$$\begin{aligned}\sigma(\hat{H}_{\pm}(\zeta;0,0)) &= \{\varepsilon\sqrt{2k|B_{\pm}| + m_0^2} : \varepsilon \in \{-1,1\}, k \in \mathbb{N}_+\} \bigcup \{m_0 \operatorname{sgn}(B_{\pm})\} \\ &=: \{\tilde{\nu}_{k,\pm} : k \in \mathbb{Z}\}.\end{aligned}$$

Note that $|\tilde{\nu}_{k,\pm}| \geq |m_0| > 0$ for all k.

1. Suppose $B_- < 0 < B_+$. Recall that $\{\mu_j(\zeta;\lambda)\}_{j\in\mathbb{Z}}$ denotes the (holomorphic in $(\zeta;\lambda)$) eigenvalues of $\hat{H}(\zeta;\lambda)$. Then there is a bijection $\iota : \mathbb{Z} \to \mathbb{Z} \times \{+,-\}$ such that $\lim_{\zeta\to\infty} \mu_j(\zeta;0,0) = \tilde{\nu}_{\iota(j)}$ for all $j \in \mathbb{Z}$. Lemma 3.1.7 asserts that $|\mu_j(\zeta;0,0)| \to \infty$ as $\zeta \to -\infty$. Hence Lemma 3.1.9 implies that $\mu_{j,-\infty}(0,0) = \pm\infty$ if and only if $\pm\tilde{\nu}_{\iota(j)} > 0$. That is, the levels $\tilde{\nu}_{\iota(j)} > 0$ correspond to branches $\mu_j(\cdot\,;0,0)$ that go to $+\infty$ at $-\infty$, while the levels $\tilde{\nu}_{\iota(j)} < 0$ correspond to branches $\mu_j(\cdot\,;0,0)$ that go to $-\infty$ at $-\infty$. Thus 0 (or any value in $(-|m_0|,|m_0|)$) separates the branches $\mu_j(\cdot\,;0,0)$ that go to $+\infty$ at $-\infty$ from those that go to $-\infty$ at $-\infty$, as demonstrated by Figure 3.1 (bottom right panel).

   We now analyze the spectrum of $\hat{H}(\zeta;\lambda)$ as λ is continuously deformed from $(0,0)$ to $(1,0)$ to $(1,1)$, thus separating the effects of m and V. Note that we can choose m_0 such that the spectral flow of H through α is well defined when $\lambda \in \{(0,0),(1,0)\}$ (by definition the spectral flow is well defined when $\lambda = (1,1)$). We follow the convention that $\mu_j(\zeta;\lambda) < \mu_{j+1}(\zeta;\lambda)$ and $\mu_{1,\infty}(0,0) = |m_0|$. This means $\mu_{j,\infty}(0,0) > 0$ and $\mu_{j,-\infty}(0,0) = +\infty$ for all $j > 0$, while $\mu_{j,\infty}(0,0) < 0$ and $\mu_{j,-\infty}(0,0) = -\infty$ for all $j \leq 0$. From (3.1.6), it follows that for all $\lambda \in [0,1]^2$, $\mu_{j,-\infty}(\lambda) = +\infty$

for all $j > 0$ and $\mu_{j,-\infty}(\lambda) = -\infty$ for all $j \leq 0$. Moreover, (3.1.6) implies that $\mu_{1,\infty}(1,0) = \max\{m_+, m_-\}$ and $\mu_{0,\infty}(1,0) = \min\{m_+, m_-\}$. By Lemma 3.1.6, the values $\mu_{j,\infty}(1,0)$ can be read off directly from (3.1.3) with $V_\pm = 0$, as they are exactly the elements of $\sigma(\hat{H}_+(0;1,0)) + \sigma(\hat{H}_-(0;1,0)$ (in increasing order with the limit of μ_1 already determined above). This confirms Theorem 3.1.1 in the case that $V \equiv 0$.

Now we set $\lambda_1 = 1$ and analyze the transition of λ_2 from 0 to 1. Let $\{\nu_{0,i,\pm}\}_{i\in\mathbb{Z}}$ denote the eigenvalues of $\hat{H}_\pm(\zeta;1,0)$, where $\nu_{0,i,\pm} < \nu_{0,i+1,\pm}$ for all $i \in \mathbb{Z}$. The eigenvalues of $\hat{H}_\pm(\zeta;1,\lambda_2)$ are then given by $\nu_{i,\pm}(\lambda_2) := \nu_{0,i,\pm} + \lambda_2 V_\pm$ for $i \in \mathbb{Z}$. To each $\nu_{i,\pm}(\lambda_2)$ is associated a unique index $j = j(\lambda_2, i, \pm)$ such that $\mu_{j(\lambda_2,i,\pm),\infty}(1,\lambda_2) = \nu_{i,\pm}(\lambda_2)$. Let $\varepsilon_{i,\pm}(\lambda_2) \in \{1,-1\}$ such that $\varepsilon_{i,\pm}(\lambda_2) = 1$ if and only if $\mu_{j(\lambda_2,i,\pm),-\infty}(1,\lambda_2) = +\infty$. It follows that

$$\begin{aligned}&\mathrm{SF}(H(1,\lambda_2);\alpha) = \\ &\quad\sum_{\delta\in\{+,-\}} \left(|\{i : \nu_{i,\delta}(\lambda_2) > \alpha,\ \varepsilon_{i,\delta}(\lambda_2) = -1\}| - |\{i : \nu_{i,\delta}(\lambda_2) < \alpha,\ \varepsilon_{i,\delta}(\lambda_2) = 1\}|\right).\end{aligned} \tag{3.1.7}$$

By (3.1.6), we know that if $\nu_{i,+}(\lambda_2) \notin \{\nu_{i,-}(\lambda_2)\}_{i\in\mathbb{Z}}$ for all λ_2 in an open interval (a,b), then $\varepsilon_{i,+}(\lambda_2)$ is constant over $\lambda_2 \in (a,b)$. For values λ_2^* and indices i,j such that $\nu_{i,+}(\lambda_2^*) = \nu_{j,-}(\lambda_2^*)$, Lemma 3.1.3 implies that $\varepsilon_{i,+}(\lambda_2)$ and $\varepsilon_{j,-}(\lambda_2)$ trade signs across λ_2^*; that is, $\varepsilon_{i,+}(\lambda_2^* + \eta) = \varepsilon_{j,-}(\lambda_2^* - \eta)$ and $\varepsilon_{j,-}(\lambda_2^* + \eta) = \varepsilon_{i,+}(\lambda_2^* - \eta)$ for all $\eta > 0$ sufficiently small. But this trade of signs has no effect on the spectral flow (i.e. if $\lim_{\zeta\to\infty} \tilde{\mu}_1(\zeta) = 1$ and $\lim_{\zeta\to\infty} \tilde{\mu}_0(\zeta) = -1$ for some smooth branches of spectrum $\tilde{\mu}_1$ and $\tilde{\mu}_0$, then any spectral flow is independent of whether $\lim_{\zeta\to-\infty}(\tilde{\mu}_1(\zeta), \tilde{\mu}_0(\zeta)) = (+\infty, -\infty)$ or $\lim_{\zeta\to-\infty}(\tilde{\mu}_1(\zeta), \tilde{\mu}_0(\zeta)) = (-\infty, +\infty)$). This means that when evaluating the right-hand side of (3.1.7), we can replace $\varepsilon_{i,\delta}(\lambda_2)$ by $\varepsilon_{i,\delta}(0)$ to obtain

$$\mathrm{SF}(H(1,1);\alpha) = \sum_{\delta\in\{+,-\}} (|\{i \le 0 : \nu_{0,i,\delta} > \alpha - V_\delta\}| - |\{i > 0 : \nu_{0,i,\delta} < \alpha - V_\delta\}|),$$

where we use the convention that $\varepsilon_{i,\pm}(0) = 1$ if and only if $i > 0$. To verify that the above expression yields Theorem 3.1.1 is a straightforward but tedious exercise. We will do so assuming that $m_- < 0 < m_+$, $|m_-| \le |m_+|$ and $\alpha - V_-, \alpha - V_+ > 0$, and leave the other cases (which are handled similarly) to the reader.

Under the above assumptions, it follows that

$$\mathrm{SF}(H(1,1);\alpha) = M_0 - \sum_{\delta\in\{+,-\}} |\{i > 0 : \nu_{0,i,\delta} < \alpha - V_\delta\}| =: M_0 - M_+ - M_-, \tag{3.1.8}$$

where

$$M_0 = \begin{cases} 1, & \alpha - V_- < |m_-| \\ 0, & \text{else}, \end{cases}$$

$$M_+ = \begin{cases} 0, & \alpha - V_+ < m_+ \\ k; & \sqrt{2(k-1)B_+ + m_+^2} < \alpha - V_+ < \sqrt{2kB_+ + m_+^2}, \quad k \in \mathbb{N}_+ \end{cases}$$

and

$$M_- = \begin{cases} 0, & \alpha - V_- < \sqrt{2|B_-| + m_-^2} \\ k; & \sqrt{2k|B_-| + m_-^2} < \alpha - V_- < \sqrt{2(k+1)|B_-| + m_-^2}, \quad k \in \mathbb{N}_+. \end{cases}$$

We will now show that (3.1.8) agrees with Theorem 3.1.1. Simplifying the formula (3.1.2) from Theorem 3.1.1, we obtain that

$$N(H_+;\alpha) = \begin{cases} 0; & \alpha - V_+ < \sqrt{2B_+ + m_+^2}, \\ k; & \sqrt{2kB_+ + m_+^2} < \alpha - V_+ < \sqrt{2(k+1)B_+ + m_+^2}, \quad k \in \mathbb{N}_+ \end{cases}$$

and

$$N(H_-;\alpha) = \begin{cases} 0; & \alpha - V_- < \sqrt{2|B_-| + m_-^2}, \\ k; & \sqrt{2k|B_-| + m_-^2} < \alpha - V_- < \sqrt{2(k+1)|B_-| + m_-^2}, \quad k \in \mathbb{N}_+. \end{cases}$$

Note from (3.1.1) that in our case,

$$\begin{aligned} I(H_+;\alpha) &= \operatorname{sgn}(\alpha - V_+ - m_+)(N(H_+;\alpha) + \frac{1}{2}), \\ I(H_-;\alpha) &= -\operatorname{sgn}(\alpha - V_- + m_-)(N(H_-;\alpha) + \frac{1}{2}). \end{aligned}$$

Observe that $N(H_\pm;\alpha) = 0$ if $\operatorname{sgn}(\alpha - V_\pm \mp m_\pm) < 0$, hence

$$I(H_+;\alpha) = \begin{cases} N(H_+;\alpha) + \frac{1}{2}, & \alpha - V_+ - m_+ > 0 \\ -\frac{1}{2}, & \alpha - V_+ - m_+ < 0 \end{cases}$$

and

$$I(H_-;\alpha) = \begin{cases} -N(H_-;\alpha) - \frac{1}{2}, & \alpha - V_- + m_- > 0 \\ \frac{1}{2}, & \alpha - V_- + m_- < 0. \end{cases}$$

Observe that $N(H_-;\alpha) = M_-$ and

$$N(H_+;\alpha) = \begin{cases} M_+, & \alpha - V_+ < m_+ \\ M_+ - 1, & \text{else.} \end{cases}$$

Thus

$$I(H_+;\alpha) = \begin{cases} M_+ - \frac{1}{2}, & \alpha - V_+ - m_+ > 0 \\ -\frac{1}{2}, & \alpha - V_+ - m_+ < 0 \end{cases}$$

and

$$I(H_-;\alpha) = \begin{cases} -M_- - \frac{1}{2}, & \alpha - V_- + m_- > 0 \\ \frac{1}{2}, & \alpha - V_- + m_- < 0. \end{cases}$$

Since $M_\pm = 0$ whenever $\alpha - V_\pm \mp m_\pm < 0$, we conclude that

$$I(H_-;\alpha) - I(H_+;\alpha) = \begin{cases} -M_- - M_+, & \alpha - V_- + m_- > 0, \\ -M_- - M_+ + 1, & \alpha - V_- + m_- < 0. \end{cases}$$

This agrees with (3.1.8), as desired.

2. Suppose $0 < B_+, B_-$. The argument is similar to case 1, only now each $\mu(\zeta;\lambda)$ converges also as $\zeta \to -\infty$. By Lemmas 3.1.3 and 3.1.9, we know that the branch $\mu(\zeta;0,0)$ that converges to m_0 as $\zeta \to -\infty$ also converges to m_0 as $\zeta \to +\infty$. Thus (3.1.6) implies that the branch $\mu(\zeta;1,0)$ that converges to m_- as $\zeta \to -\infty$ must converge to m_+ as $\zeta \to +\infty$. Finally, this implies that the branch $\mu(\zeta;1,1)$ that converges to $m_- + V_-$ as $\zeta \to -\infty$ must converge to $m_+ + V_+$ as $\zeta \to \infty$, and the result follows.

The case $B_+ < 0 < B_-$ is handled similarly to case 1; the case $B_+, B_- < 0$ is handled similarly to case 2. This completes the result. $\square$

3.2 Physical observable

Let $P(y) = P \in \mathfrak{S}(0,1)$ and $\varphi \in \mathfrak{S}(0,1; E_1, E_2)$ for some $[E_1, E_2] \subset \mathcal{R}$. As in (1.0.1) and Section 2, define the interface conductivity associated to H in (3.0.2) by

$$\sigma_I := \operatorname{Tr} i[H,P]\varphi'(H). \tag{3.2.1}$$

The goal of this section is to relate σ_I to the spectral flow from Section 3.1, and to prove its stability with respect to perturbations of H. To do so, it is convenient to use the framework of pseudo-differential operators (ΨDOs) and the Helffer-Sjöstrand formula; the notation and main results we need are summarized in Appendix A.1. Let

$$\sigma(x,\xi,\zeta) := \xi\sigma_1 + (\zeta - A_2(x))\sigma_2 + m(x)\sigma_3 + V(x)\sigma_0$$

denote the *Weyl symbol* of H (so that $H = \operatorname{Op}(\sigma)$). Similarly, define

$$\sigma_\pm(x,\xi,\zeta) := \xi\sigma_1 + (\zeta - xB_\pm)\sigma_2 + m_\pm\sigma_3 + V_\pm\sigma_0$$

so that $H_\pm = \operatorname{Op}(\sigma_\pm)$. Note that as opposed to the setting described by (H1), the symbols $\sigma_\pm$ still depend on the spatial variable x to model a constant magnetic field.

As mentioned at the beginning of this section, σ is not elliptic because its eigenvalues can remain small even as x and ζ get large. Still, using the fact that

$$\sigma^2(x,\xi,\zeta) = \xi^2 + (\zeta - A_2(x))^2 + m^2(x) + V^2(x) + 2V(x)(\xi\sigma_1 + (\zeta - xB_\pm)\sigma_2 + m_\pm\sigma_3),$$

we obtain that

$$|\det \sigma(x,\xi,\zeta)|^{1/2} \geq c_1\langle \xi, \zeta - A_2(x)\rangle - c_2 \tag{3.2.2}$$

for some $0 < c_1 < 1$ and $c_2 > 0$. In order to make use of this inequality, we need to verify

Lemma 3.2.1. *The map* $(x,\xi,\zeta) \mapsto \langle \xi, \zeta - A_2(x)\rangle$ *is an order function.*

We refer to Section A.1 for the definitions of an order function and $\langle\cdot\rangle$.

Proof. It is known (see e.g. [89]) that $\mathbb{R}^2 \ni Y \mapsto \langle Y\rangle$ is an order function. Thus there exist positive constants C_0 and N_0 such that

$$\langle \xi_1, \zeta_1 - A_2(x_1)\rangle \leq C_0\langle \xi_2 - \xi_1, \zeta_2 - A_2(x_2) - (\zeta_1 - A_2(x_1))\rangle^{N_0}\langle \xi_2, \zeta_2 - A_2(x_2)\rangle$$

for all $(x_1,\xi_1,\zeta_1),(x_2,\xi_2,\zeta_2) \in \mathbb{R}^3$. We write

$$(\zeta_2 - A_2(x_2) - (\zeta_1 - A_2(x_1)))^2 \leq 2((\zeta_2 - \zeta_1)^2 + (A_2(x_2) - A_2(x_1))^2,$$

and seek to bound the second term on the above right-hand side. We have

$$\begin{aligned}(A_2(x_2) - A_2(x_1))^2 &= (x_2B(x_2) - x_1B(x_1))^2 = ((x_2 - x_1)B(x_2) + x_1(B(x_2) - B(x_1)))^2\\ &\leq 2\,\|B\|_\infty^2\,(x_2 - x_1)^2 + 2x_1^2(B(x_2) - B(x_1))^2.\end{aligned}$$

Since $B(x_2)-B(x_1)$ vanishes whenever x_1 and x_2 are sufficiently large and of the same sign, there exist positive constants C_1 and C_2 such that $x_1^2(B(x_2)-B(x_1))^2 \leq C_1(x_2-x_1)^2+C_2$. We conclude that

$$\langle \xi_2 - \xi_1, \zeta_2 - A_2(x_2) - (\zeta_1 - A_2(x_1))\rangle \leq C\langle x_2 - x_1, \xi_2 - \xi_1, \zeta_2 - \zeta_2\rangle$$

for some $C > 0$, and the result is complete. $\square$

We begin by showing that σ_I is well defined. To do this, we will need two useful decay properties for symbols of related operators.

Lemma 3.2.2. *If $z \in \mathbb{C}$ such that $\Im z \neq 0$, then $(z - H)^{-1} = \mathrm{Op}(r_z)$ for some $r_z \in S(\langle \xi, \zeta - A_2(x) \rangle^{-1})$.*

Note that $S(\langle \xi, \zeta - A_2(x) \rangle^{-1})$ is well defined, by Lemma 3.2.1.

Proof. Since H is self-adjoint, we know that $(z-H)^{-1}$ is well defined and bounded. To obtain bounds for the symbol of $(z - H)^{-1}$ (and show that it is a ΨDO in the first place), we use Beals's criterion presented in [34, Proposition 8.3]. This result states that $(z-H)^{-1} = \mathrm{Op}(r_z)$ for some $r_z \in S(1)$ if and only if for any collection of linear forms

$$\ell_1(x, y, \xi, \zeta), \ell_2(x, y, \xi, \zeta), \ldots, \ell_N(x, y, \xi, \zeta)$$

on $\mathbb{R}^4$, the operator $ad_{L_1} \circ \cdots \circ ad_{L_N} \circ (z - H)^{-1}$ is bounded in $L^2(\mathbb{R}^2) \otimes \mathbb{C}^2$, where $L_j := \mathrm{Op}(\ell_j)$ and $ad_A B := [A, B]$. Since $\sigma_\xi = \sigma_1$ and $\sigma_\zeta = \sigma_2$ are constant and σ_x is bounded, it is clear that $[L_j, H]$ is bounded for any such L_j. Thus the identity $[\mathcal{O}, (z - H)^{-1}] = (z - H)^{-1}[\mathcal{O}, H](z - H)^{-1}$ easily implies that $(z - H)^{-1} = \mathrm{Op}(r_z)$ for some $r_z \in S(1)$.

By (3.2.2) and the composition calculus, we have

$$(z - \sigma)\sharp(z - \sigma)^{-1} = 1 + b_z,$$

where $b_z \in S(\langle \xi, \zeta - A_2(x) \rangle^{-2})$. Indeed, all derivatives of σ are bounded and $(z - \sigma)^{-1} \in S(\langle \xi, \zeta - A_2(x) \rangle^{-1})$. Letting $G_z := \mathrm{Op}((z - \sigma)^{-1})$ and $B_z := \mathrm{Op}(b_z)$, this means

$$(z - H)G_z = 1 + B_z.$$

Applying $(z-H)^{-1}$ to both sides (on the left), we get

$$(z-H)^{-1} = G_z - (z-H)^{-1}B_z.$$

The first term on the right-hand side has symbol in $S(\langle \xi, \zeta - A_2(x)\rangle^{-1})$ and the second term has symbol in $S(\langle \xi, \zeta - A_2(x)\rangle^{-2}) \subset S(\langle \xi, \zeta - A_2(x)\rangle^{-1})$. Therefore, $r_z \in S(\langle \xi, \zeta - A_2(x)\rangle^{-1})$ as desired. $\square$

Lemma 3.2.3. *For any $\Phi \in \mathcal{C}_c^\infty(E_1, E_2)$, we have $\Phi(H) \in \mathrm{Op}(S(\langle x, \xi, \zeta\rangle^{-\infty}))$.*

Proof. For any $p > 0$, we can write $\Phi(H) = (i-H)^{-p}\Phi_p(H)$ with $\Phi_p \in \mathcal{C}_c^\infty(E_1, E_2)$. By Lemma 3.2.2 and the composition calculus, this means $\Phi(H) \in \mathrm{Op}(S(\langle \xi, \zeta - A_2(x)\rangle^{-\infty}))$. Since $H_\pm$ has a spectral gap in $[E_1, E_2]$, we know that $\Phi(H_\pm) = 0$. Thus we can write $\Phi(H) = \phi(x)(\Phi(H) - \Phi(H_+)) + (1-\phi(x))(\Phi(H) - \Phi(H_-))$, for some $\phi \in \mathfrak{S}(0,1)$. The Helffer-Sjöstrand formula (A.1.6) implies that

$$\Phi(H) - \Phi(H_+) = \frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\Phi}(z)(z-H)^{-1}(H-H_+)(z-H_+)^{-1} d^2 z.$$

Since $\sigma - \sigma_+$ vanishes whenever x is sufficiently large, it follows that $\Phi(H) - \Phi(H_+) \in \mathrm{Op}(S(\langle x_+\rangle^{-\infty}))$, where $x_+ := \max\{x, 0\}$. Since ϕ vanishes whenever $-x$ is sufficiently large, we conclude that $\phi(x)(\Phi(H) - \Phi(H_+)) \in \mathrm{Op}(S(\langle x\rangle^{-\infty}))$. The same reasoning shows that $(1-\phi(x))(\Phi(H) - \Phi(H_-)) \in \mathrm{Op}(S(\langle x\rangle^{-\infty}))$. We have thus shown that $\Phi(H) \in \mathrm{Op}(S(\langle \xi, \zeta - A_2(x)\rangle^{-\infty}) \cap S(\langle x\rangle^{-\infty}))$. By interpolation, the result is complete. $\square$

Lemma 3.2.4. *For any $\Phi \in \mathcal{C}_c^\infty(E_1, E_2)$, the operator $[H, P]\Phi(H)$ is trace-class.*

Proof. We have $[H, P] = -iP'(y)\sigma_2$ with $P' \in \mathcal{C}_c^\infty$, hence $[H, P] \in \mathrm{Op}(S(\langle y\rangle^{-\infty}))$. The result then follows from Lemma 3.2.3 and the composition calculus. $\square$

Now that we have shown that σ_I is well defined, we relate it to the spectral flow.

Theorem 3.2.5. *For any $\alpha \in [E_1, E_2]$, we have $2\pi\sigma_I = SF(H; \alpha)$.*

Combining Theorems 3.1.1 and 3.2.5, we obtain an explicit formula for σ_I. In particular, σ_I is quantized and independent of compact perturbations in m, B, and V. Moreover, σ_I is stable with respect to sufficiently small changes in $m_\pm, B_\pm$ and $V_\pm$.

Proof. We follow the arguments presented in [10, Section A]. Recall Lemmas 3.1.3 and 3.1.4, which state that the spectrum of $\hat{H}(\zeta)$ for $\zeta \in \mathbb{R}$ consists entirely of simple eigenvalues $\{\mu_j(\zeta)\}_{j\in\mathbb{Z}}$, where each $\mu_j : \mathbb{R} \to \mathbb{R}$ is analytic. For $j \in \mathbb{Z}$, let $\psi_j(\cdot, \zeta)$ denote the normalized eigenfunction (unique up to a phase) of $\hat{H}(\zeta)$ corresponding to eigenvalue $\mu_j(\zeta)$. Using Lemma 3.1.8, let $\mathcal{J} \subset \mathbb{Z}$ be the finite set of indices corresponding to branches μ_j that ever enter the interval $[E_1, E_2]$. For any $\Phi \in \mathcal{C}_c^\infty(E_1, E_2)$, the Schwartz kernel (see Section A.1) of $\Phi(H)$ is thus given by

$$k_\Phi(x, x'; y - y') = \int_{\mathbb{R}} \sum_{j\in\mathcal{J}} \Phi(\mu_j(\zeta))\psi_j(x, \zeta)\psi_j^*(x', \zeta)\frac{e^{i(y-y')\zeta}}{2\pi}d\zeta. \tag{3.2.3}$$

Lemmas 3.1.6 and 3.1.7 imply that each $\mu_j(\zeta)$ escapes $[E_1, E_2]$ whenever $|\zeta|$ is sufficiently large, hence the integrand in (3.2.3) is compactly supported in ζ.

By Lemma 2.1.2, we obtain that $\sigma_I = \operatorname{Tr} i[\Psi(H), P]\varphi'(H)$ for any $\Psi \in \mathcal{C}_c^\infty(E_1, E_2)$ that satisfies $\Psi(\lambda) = \lambda$ for all λ in some open interval containing $\operatorname{supp}(\varphi')$. The kernel of $[\Psi(H), P]\varphi'(H)$ is

$$t(x, x'; y, y') = \int_{\mathbb{R}^2} (P(y'') - P(y))k_\Psi(x, x''; y - y'')k_{\varphi'}(x'', x'; y'' - y')dx''dy'',$$

where k_Φ for $\Phi \in \mathcal{C}_c^\infty(E_1, E_2)$ is given by (3.2.3). It follows from (A.1.7) that

$$\begin{aligned}\sigma_I &= i \operatorname{tr} \int_{\mathbb{R}^2} t(x, x; y, y)dxdy \\ &= i \operatorname{tr} \int_{\mathbb{R}^4} (P(y') - P(y))k_\Psi(x, x'; y - y')k_{\varphi'}(x', x; y' - y)dx'dy'dxdy.\end{aligned}$$

Changing integration variables $(y,y') \to (z,y')$ with $z = y - y'$, and using that $\int_{\mathbb{R}} P(y') - P(y'+z)dy' = -z$ (which follows from $P \in \mathfrak{S}(0,1)$), we obtain

$$\sigma_I = -i \operatorname{tr} \int_{\mathbb{R}^3} z k_\Psi(x,x';z) k_{\varphi'}(x',x;-z) dx' dx dz.$$

By Parseval and using that $k^*_{\varphi'}(x,x';z) = k_{\varphi'}(x',x;-z)$, we have

$$\sigma_I = \frac{1}{2\pi} \operatorname{tr} \int_{\mathbb{R}^3} \partial_\zeta \hat{k}_\Psi(x,x';\zeta) \hat{k}^*_{\varphi'}(x,x',\zeta) dx' dx d\zeta.$$

Note that for any $\Phi \in \mathcal{C}_c^\infty(E_1,E_2)$,

$$\hat{k}_\Phi(x,x';\zeta) = \sum_{j=1}^{J} \Phi(\mu_j(\zeta)) \psi_j(x,\zeta) \psi_j^*(x',\zeta),$$

hence

$$2\pi\sigma_I = \operatorname{tr} \int_{\mathbb{R}^3} \sum_{j,k=1}^{J} \partial_\zeta (\Psi(\mu_j(\zeta)) \psi_j(x,\zeta) \psi_j^*(x',\zeta)) \varphi'(\mu_k(\zeta)) \psi_k(x',\zeta) \psi_k^*(x,\zeta) dx' dx d\zeta. \tag{3.2.4}$$

Since

$$\begin{aligned}
&\operatorname{tr} \int_{\mathbb{R}^2} \partial_\zeta (\psi_j(x,\zeta) \psi_j^*(x',\zeta)) \psi_k(x',\zeta) \psi_k^*(x,\zeta) dx' dx \\
&= \delta_{jk} \Big(\int_{\mathbb{R}} \psi_k^*(x,\zeta) \partial_\zeta \psi_k(x,\zeta) dx + \int_{\mathbb{R}} \partial_\zeta \psi_k^*(x,\zeta) \psi_k(x,\zeta) dx \Big) \\
&= \delta_{jk} \partial_\zeta \int_{\mathbb{R}} \psi_k^*(x,\zeta) \psi_k(x,\zeta) dx = 0,
\end{aligned}$$

the contribution to (3.2.4) from $\partial_\zeta(\psi_j(x,\zeta)\psi_j^*(x',\zeta))$ vanishes, and thus

$$2\pi\sigma_I = \operatorname{tr}\int_{\mathbb{R}^3}\sum_{j,k=1}^{J}\partial_\zeta\Psi(\mu_j(\zeta))\psi_j(x,\zeta)\psi_j^*(x',\zeta)\varphi'(\mu_k(\zeta))\psi_k(x',\zeta)\psi_k^*(x,\zeta)dx'dxd\zeta$$
$$= \int_{\mathbb{R}}\sum_{j=1}^{J}\partial_\zeta\Psi(\mu_j(\zeta))\varphi'(\mu_j(\zeta))d\zeta = \int_{\mathbb{R}}\sum_{j=1}^{J}\partial_\zeta\mu_j(\zeta)\varphi'(\mu_j(\zeta))d\zeta = \sum_{j=1}^{J}\int_{\mathbb{R}}\partial_\zeta\varphi(\mu_j(\zeta))d\zeta,$$

where we have used orthonormality of the eigenfunctions to justify the second equality above. It follows that

$$2\pi\sigma_I = \sum_{j=1}^{J}\Big(\lim_{\zeta\to+\infty}\varphi(\mu_j(\zeta)) - \lim_{\zeta\to-\infty}\varphi(\mu_j(\zeta))\Big).$$

Since $\varphi \in \mathfrak{S}(0,1;E_1,E_2)$, the above right-hand side is indeed well defined and the result is complete. □

Now we want to analyze the stability of σ_I with respect to perturbations. Let

$$H_\mu = H + \mu W \quad \text{for} \quad \mu \in [0,1],$$

where W is a symmetric ΨDO. We begin with a criterion for stability of σ_I. It will require two preliminary results (Lemmas 3.2.7 and 3.2.8). Below, U° denotes the interior of U.

Theorem 3.2.6. *Let $\Psi \in \mathcal{C}_c^\infty(E_1,E_2)$ such that $\varphi' \in \mathcal{C}_c^\infty(\{\Psi(\lambda)=\lambda\}^\circ)$. If H_μ is self-adjoint and the operators $[H_\mu,P]\varphi'(H_\mu)$, $\varphi'(H_\mu)-\varphi'(H_0)$ and $\Psi(H_\mu)-\Psi(H_0)$ are trace-class, then $\sigma_I(H_\mu)=\sigma_I(H_0)$.*

Proof. By assumption, $\sigma_I(H_\mu)$ is well defined. As in the proof of Theorem 3.2.5, it follows that $\sigma_I(H_\lambda) = \operatorname{Tr} i[\Psi(H_\lambda),P]\varphi'(H_\lambda)$ for $\lambda \in \{0,\mu\}$. We can thus write the difference of conductivities as

$$\sigma_I(H_\mu) - \sigma_I(H_0) = \operatorname{Tr} i[\Psi(H_\mu), P](\varphi'(H_\mu) - \varphi'(H_0)) + \operatorname{Tr} i[\Psi(H_\mu) - \Psi(H_0), P]\varphi'(H_0),$$

where our hypotheses have guaranteed that each trace is well defined. Using Lemma 3.2.7, we can replace P above by P_{y_0}, where $P_{y_0}(y) := P(y - y_0)$. Again applying cyclicity (and linearity) of the trace, we get $\sigma_I(H_\mu) - \sigma_I(H_0) = \sum_{j=1}^4 \operatorname{Tr} P_{y_0} A_j$, where the A_j are all trace-class. The result then follows from Lemma 3.2.8. $\square$

Lemma 3.2.7. *Let $P_1, P_2 \in \mathfrak{S}(0,1)$ with $P_j = P_j(y)$. Then*

$$\operatorname{Tr} i[H, P_1]\varphi'(H) = \operatorname{Tr} i[H, P_2]\varphi'(H).$$

Proof. With Ψ defined in Theorem 3.2.6, we have

$$\operatorname{Tr} i[H, P_2]\varphi'(H) - \operatorname{Tr} i[H, P_1]\varphi'(H) = \operatorname{Tr} i[\Psi(H), P_2 - P_1]\varphi'(H).$$

Since $P_2 - P_1 \in \langle x\rangle^{-\infty}$, Lemma 3.2.3 implies that $(P_2 - P_1)\varphi'(H)$ is trace-class. Therefore,

$$\begin{aligned}\operatorname{Tr} i[\Psi(H), P_2 - P_1]\varphi'(H) &= \operatorname{Tr} i\Psi(H)(P_2 - P_1)\varphi'(H) - \operatorname{Tr} i(P_2 - P_1)\Psi(H)\varphi'(H)\\ &= \operatorname{Tr} i(P_2 - P_1)\varphi'(H)\Psi(H) - \operatorname{Tr} i(P_2 - P_1)\Psi(H)\varphi'(H) = 0,\end{aligned}$$

where we have used cyclicity of the trace to justify the second line, and the fact that $[\varphi'(H), \Psi(H)] = 0$ for the last line. $\square$

Lemma 3.2.8. *Let $P(y) = P \in \mathfrak{S}(0,1)$ and $y_0 \in \mathbb{R}$, and define $P_{y_0}(y) := P(y - y_0)$. Then for any trace-class operator A on $L^2(\mathbb{R}^2) \otimes \mathbb{C}^n$, we have $\operatorname{Tr} P_{y_0} A \to 0$ as $y_0 \to \infty$.*

Proof. Writing $A = \frac{1}{2}(A + A^*) + \frac{1}{2}(A - A^*)$, with $\frac{1}{2}(A + A^*)$ and $\frac{i}{2}(A - A^*)$ trace-class and self-adjoint and using the triangle inequality, we may assume that A is self-adjoint. Fix $\varepsilon > 0$.

By the spectral theorem, there exists an orthonormal basis $\{\psi_j\}_{j=1}^{\infty}$ of $L^2(\mathbb{R}^2)\otimes\mathbb{C}^n$ such that $A\psi_j = \lambda_j\psi_j$, with $\{\lambda_j\}_{j=1}^{\infty} \subset \mathbb{R}$ satisfying $\sum_{j=1}^{\infty} |\lambda_j| < \infty$. Thus there exists $N \in \mathbb{N}$ such that $\sum_{j=N}^{\infty} |(\psi_j, P_{y_0}A\psi_j)| \leq \sum_{j=N}^{\infty} |\lambda_j| < \varepsilon/2$ for all $y_0 \in \mathbb{R}$. Since $\{\psi_j\}_{j=1}^{\infty} \subset L^2(\mathbb{R}^2)\otimes\mathbb{C}^n$, we know that, for y_0 sufficiently large, $\left\|P_{y_0}\psi_j\right\| < \varepsilon/\left(2N\left\|A\right\|\right)$ for all $j \in \{1, 2, \ldots, N-1\}$. It follows that $|\operatorname{Tr} P_{y_0}A| \leq \sum_{j=1}^{\infty} |(\psi_j, P_{y_0}A\psi_j)| < \varepsilon$ for all y_0 sufficiently large. □

We now use Theorem 3.2.6 to prove stability of σ_I under a large class of perturbations W. For the rest of this section, let $\Phi_0 \in \mathcal{C}_c^\infty(E_1, E_2)$ such that $\Psi \in \mathcal{C}_c^\infty(\{\Phi_0 = 1\}^\circ)$, with Ψ as in Theorem 3.2.6.

Theorem 3.2.9. *Let W be a symmetric ΨDO, such that $(i \pm H_0)^{-1}W$ is bounded and $\Phi_0(H_0)W$ is trace-class. Then $\sigma_I(H_\mu) = \sigma_I(H_0)$ for all $\mu > 0$ sufficiently small.*

Proof. We verify the assumptions of Theorem 3.2.6. Since $(i \pm H_0)^{-1}W$ is bounded, $i \pm H_\mu : (i - H_0)^{-1}\mathcal{H} \to \mathcal{H}$ is bijective whenever $\mu < \left\|(i \pm H_0)^{-1}W\right\|^{-1}$, with $(i \pm H_\mu)^{-1} = (1 \pm \mu(i \pm H_0)^{-1}W)^{-1}(i \pm H_0)^{-1}$. Hence for all $\mu > 0$ sufficiently small, H_μ is self-adjoint with the same domain of definition $\mathcal{D}(H_\mu) = \mathcal{D}(H_0) = (i - H_0)^{-1}\mathcal{H}$.

It remains to verify that $[H_\mu, P]\varphi'(H_\mu)$ and $\Phi(H_\mu) - \Phi(H_0)$ are trace-class for $\Phi \in \{\varphi', \Psi\}$. We start with the difference

$$\begin{aligned}\Phi(H_\mu) - \Phi(H_0) = (\Phi(H_\mu) - \Phi(H_0))(\Phi_0(H_\mu) - \Phi_0(H_0))\\ + \Phi(H_0)(\Phi_0(H_\mu) - \Phi_0(H_0)) + (\Phi(H_\mu) - \Phi(H_0))\Phi_0(H_0),\end{aligned}$$

which can be rearranged to give

$$\begin{aligned}&(\Phi(H_\mu) - \Phi(H_0))(1 - (\Phi_0(H_\mu) - \Phi_0(H_0)))\\ &\qquad = \Phi(H_0)(\Phi_0(H_\mu) - \Phi_0(H_0)) + (\Phi(H_\mu) - \Phi(H_0))\Phi_0(H_0).\end{aligned} \tag{3.2.5}$$

By the Helffer-Sjöstrand formula,

$$\Phi_0(H_\mu) - \Phi_0(H_0) = \frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\Phi}_0(z)(z-H_0)^{-1}\mu W(z-H_\mu)^{-1}d^2z. \tag{3.2.6}$$

Recall that $\tilde{\Phi}_0 \in \mathcal{C}_c^\infty(\mathbb{C})$ with $|\bar{\partial}\tilde{\Phi}_0(z)| \le C|\Im z|^2$, and write

$$(z-H_0)^{-1} = (1+(i-z)(z-H_0)^{-1})(i-H_0)^{-1}.$$

Since $\left\|(z-H_\mu)^{-1}\right\| \le |\Im z|^{-1}$, we see that the norm of $\Phi_0(H_\mu) - \Phi_0(H_0)$ is bounded by $C\mu$, meaning that it is less than 1 for all μ small enough. It thus suffices to show that each term on the right-hand side of (3.2.5) is trace-class, as $1-(\Phi_0(H_\mu)-\Phi_0(H_0))$ has bounded inverse. Using (3.2.6), the first term becomes

$$\Phi(H_0)(\Phi_0(H_\mu) - \Phi_0(H_0)) = \frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\Phi}_0(z)(z-H_0)^{-1}\mu\Phi(H_0)W(z-H_\mu)^{-1}d^2z. \tag{3.2.7}$$

By our assumption that $\Phi(H_0)W$ is trace-class (and again using that all singularities of the resolvent operators are compensated by the decay in $\bar{\partial}\tilde{\Phi}_0$), we conclude that (3.2.7) is trace-class. Applying the same argument to the second term

$$(\Phi(H_\mu) - \Phi(H_0))\Phi_0(H_0) = -\frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\Phi}(z)(z-H_\mu)^{-1}\mu W\Phi_0(H_0)(z-H_0)^{-1}d^2z, \tag{3.2.8}$$

it follows that $\Phi(H_\mu) - \Phi(H_0)$ is trace-class.

For the first operator, we write

$$[H_\mu, P]\Phi(H_\mu) = [H_\mu, P]\Phi(H_0) + [H_\mu, P](\Phi(H_\mu) - \Phi(H_0)), \tag{3.2.9}$$

with the first term on the above right-hand side trace-class by Lemma 3.2.3 and the composition calculus. To show that the second term is also trace-class, we again use (3.2.5).

Namely, it suffices to show that

$$T_1 := [H_0, P]A, \qquad T_2 := [W, P]A, \qquad T_3 := [H_0, P]B, \qquad T_4 := [W, P]B$$

are trace-class, with $A := \Phi(H_0)(\Phi_0(H_\mu) - \Phi_0(H_0))$ and $B := (\Phi(H_\mu) - \Phi(H_0))\Phi_0(H_0)$. That T_1 is trace-class follows immediately from (3.2.7) and boundedness of $[H_0, P] = -iP'(y)\sigma_2$. We know that PWA is trace-class (since $(i \pm H_0)^{-1}W$ is bounded; this is an assumption on W), thus T_2 is trace-class if WPA is. We write

$$\begin{aligned}
WPA &= \frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\Phi}_0(z) WP(z - H_0)^{-1}\mu\Phi(H_0)W(z - H_\mu)^{-1} d^2z \\
&= \frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\Phi}_0(z) W(z - H_0)^{-1}P\mu\Phi(H_0)W(z - H_\mu)^{-1} d^2z \\
&\quad + \frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\Phi}_0(z) W[P, (z - H_0)^{-1}]\mu\Phi(H_0)W(z - H_\mu)^{-1} d^2z.
\end{aligned}$$

Since $[P, (z - H_0)^{-1}] = -(z - H_0)^{-1}[H_0, P](z - H_0)^{-1}$, boundedness of $[H_0, P]$ and our assumption on W imply that WPA is trace-class. Using (3.2.8) and the identity

$$\begin{aligned}
(z - H_\mu)^{-1} &= (i - H_\mu)^{-1}(1 + (i - z)(z - H_\mu)^{-1}) \\
&= (i - H_0)^{-1}(1 - \mu W(i - H_0)^{-1})^{-1}(1 + (i - z)(z - H_\mu)^{-1}),
\end{aligned}$$

we similarly conclude that T_3 and T_4 are trace-class. This completes the result. $\square$

We now prove a stability result that does not require the perturbation to be “small”. To do this, we will need the stronger assumption that $(i \pm H_0)^{-1}W$ is compact.

Theorem 3.2.10. *Let W be a symmetric ΨDO. Assume that $(i \pm H_0)^{-1}W$ is compact and $\Phi_0(H_0)W$ is trace-class. Then $\sigma_I(H_1) = \sigma_I(H_0)$.*

Proof. We again verify the hypotheses of Theorem 3.2.6. The fact that $(i \pm H_0)^{-1}W$ is compact implies that $H_1 = H_0 + W$ is self-adjoint with domain of definition $\mathcal{D}(H_1) = \mathcal{D}(H_0)$.

Indeed, the fact that W is symmetric implies that the kernel of $i+H_1$ is trivial. The Fredholm alternative and our compactness assumption imply that the dimension of the kernel of $1+(i+H_0)^{-1}W$ is equal to the codimension of its range. But $1+(i+H_0)^{-1}W = (i+H_0)^{-1}(i+H_1)$ with $(i+H_0)^{-1} : \mathcal{H} \to \mathcal{D}(H_0)$ a bijection, and thus $\operatorname{codim} \operatorname{Ran}(i+H_1) = \dim\ker(i+H_1) = 0$. The same argument also shows that $\operatorname{codim} \operatorname{Ran}(i-H_1) = \dim\ker(i-H_1) = 0$. We conclude by [70, Theorem VIII.3] that H_1 is self-adjoint.

We now prove the necessary trace-class properties. Let $\Phi \in \{\varphi', \Psi\}$. By (3.2.5), (3.2.7) and (3.2.8), we have that $\Theta(1-\Theta_0)$ is trace-class, where $\Theta := \Phi(H_1) - \Phi(H_0)$ and $\Theta_0 := \Phi_0(H_1) - \Phi_0(H_0)$. We know that Θ_0 is compact by (3.2.6) and our assumption that W is relatively compact with respect to H_0. Thus there exist Θ_{00} and Θ_{01} such that Θ_{00} has finite rank, $\|\Theta_{01}\| < 1$, and $\Theta_0 = \Theta_{00} + \Theta_{01}$. It follows that $\Theta(1-\Theta_{01}) = \Theta(1-\Theta_0) + \Theta\Theta_{00}$ is trace-class. Applying $(1-\Theta_{01})^{-1}$ to both sides (on the right), we conclude that Θ is trace-class.

We now show that $[H_1, P]\Phi(H_1)$ is trace-class. Using (3.2.9), it suffices to show that $[H_1, P]\Theta$ is trace-class. The proof of Theorem 3.2.9 shows that $[H_1, P]\Theta(1-\Theta_0)$ is trace-class. As above, we write $[H_1, P]\Theta = (T + [H_1, P]\Theta\Theta_{00})(1-\Theta_{01})^{-1}$ with T and $[H_1, P]\Theta\Theta_{00}$ trace-class (the latter because Θ_{00} has finite rank) and $(1-\Theta_{01})^{-1}$ bounded. This completes the result. $\square$

Using Lemmas 3.2.2 and 3.2.3, we see that for any $p > 0$,

$$W \in \operatorname{Op}(S(\langle \xi, \zeta - A_2(x)\rangle \langle y\rangle^{-1-p}))$$

satisfies the assumptions of Theorem 3.2.9 and $W \in \operatorname{Op}(S(\langle \xi, \zeta - A_2(x)\rangle^{1-p} \langle x\rangle^{-p} \langle y\rangle^{-1-p}))$ satisfies the assumptions of Theorem 3.2.10. Note that the assumption that $\Phi_0(H_0)W$ is trace-class forces the symbol of W to decay in y, as the symbol of H_0 is independent of this variable. We now introduce two stability results that no longer require this decay in y.

Theorem 3.2.11. *Let $W = W(x, y)$ be a symmetric point-wise multiplication operator in $S(1)$ that is compactly supported in x. Then $\sigma_I(H + W) = \sigma_I(H)$.*

Proof. The same proofs of Lemmas 3.2.2 and 3.2.3 easily imply that these results hold with H replaced by $H + W$. The fact that W is bounded implies that $H + W$ is self-adjoint. Hence $H^{(\mu)} := H + \mu W$ satisfies the assumptions of Corollary 2.4.5 for all $\mu \in [0, 1]$ and the result follows. $\square$

Our next result trades the trace-class assumption of $\Phi_0(H_0)W$ in Theorem 2.1.7 for a smoothness property of W.

Theorem 3.2.12. *Let $W = \mathrm{Op}(w)$ be a symmetric ΨDO satisfying*

$$w \in S(\langle \xi, \zeta - A_2(x)\rangle^{1-\delta}\langle x, y\rangle^{-\delta})$$

for some $\delta > 0$, and $\partial_\alpha w \in S(1)$ for all $|\alpha| \geq 1$. Then $\sigma_I(H + W) = \sigma_I(H)$.

Proof. Since W is relatively compact with respect to H with the latter self-adjoint, we know that $H^{(\mu)} := H + \mu W$ is self-adjoint for all $\mu \in [0, 1]$. Following the proof of Lemma 3.2.2 and using the boundedness of $\partial_\alpha w$, we verify that $H^{(\mu)} \in \mathrm{Op}(S(\langle \xi, \zeta - A_2(x)\rangle^{-1}))$ for all μ. Thus (3.2.5) implies that $\Theta^{(\mu)}(1 - \Theta_0^{(\mu)}) \in \mathrm{Op}(S(x, \xi, \zeta)^{-\infty})$, where $\Theta^{(\mu)} := \Phi(H^{(\mu)}) - \Phi(H)$ and $\Theta_0^{(\mu)} := \Phi_0(H^{(\mu)}) - \Phi_0(H)$. The Helffer-Sjöstrand formula implies that $\Theta_0^{(\mu)} \in \mathrm{Op}(S(\langle x, y, \xi, \zeta\rangle^{-\delta}))$, and therefore $\Theta_0^{(\mu)} = \Theta_{00}^{(\mu)} + \Theta_{01}^{(\mu)}$, where $\Theta_{00}^{(\mu)} \in \mathrm{Op}(S(\langle x, y, \xi, \zeta\rangle^{-\infty}))$ and $\Theta_{01}^{(\mu)}$ has symbol in $S(1)$ as small as necessary. We conclude that $\Theta^{(\mu)} = (T + \Theta^{(\mu)}\Theta_{00}^{(\mu)})(1 - \Theta_{01}^{(\mu)})^{-1}$ with $T \in \mathrm{Op}(S(x, \xi, \zeta)^{-\infty})$, $\Theta^{(\mu)}\Theta_{00}^{(\mu)} \in \mathrm{Op}(S(\langle x, y, \xi, \zeta\rangle^{-\infty}))$ and $(1 - \Theta_{01}^{(\mu)})^{-1} \in \mathrm{Op}(S(1))$. It follows from the composition calculus that $\Phi(H^{(\mu)}) = \Phi(H) + \Theta^{(\mu)} \in \mathrm{Op}(S(\langle x, \xi, \zeta\rangle^{-\infty}))$. We have shown that $H^{(\mu)}$ satisfies the assumptions of Corollary 2.4.5 for all $\mu \in [0, 1]$, and the proof is complete. $\square$

We have provided four stability results, each of which has a different assumption on the perturbation W. We now compare these assumptions using four illustrative examples.

Example 1. Suppose $W = W(y) = \eta\langle y\rangle^{-1-\delta}$ for some $\delta > 0$, where $\eta \in \{1, -1\}$. Then Lemma 3.2.3 and the composition calculus imply that for any $p > 0$, $\Phi_0(H_0)W \in \mathrm{Op}(S(\langle y\rangle^{-1-\delta}\langle x, \xi, \zeta\rangle^{-p}))$. It follows that the symbol of $\Phi_0(H_0)W$ is integrable, meaning that $\Phi_0(H_0)W$ is trace-class. Since W is bounded, we see that W satisfies the assumptions of Theorem 3.2.9. This means $\sigma_I(H + \mu W) = \sigma_I(H)$ for all $\mu > 0$ sufficiently small. But note that $(i+H_0)^{-1}W$ is not compact, as its symbol does not decay in $\langle x, \zeta\rangle$. Thus Theorem 3.2.10 does not apply. It is also clear that Theorem 3.2.11 does not apply since W is independent of x. Theorem 3.2.12 does not apply since the symbol of $(i + H)^{-1}W$ does not decay in $\langle x, \zeta\rangle$.

Example 2. Suppose $W = W(x, y) = a\langle x, y\rangle^{-2-\delta}\,\mathrm{sgn}(y)$ for some constants $a \in \mathbb{R}$ and $\delta > 0$. Define $W_0(x, y) := a\langle x, y\rangle^{-2-\delta}$. As above it follows that $\Phi_0(H_0)W_0$ is trace-class. Since $y \mapsto \mathrm{sgn}(y)$ is bounded, we conclude that $\Phi_0(H_0)W$ is trace-class. Moreover, since W_0 decays in both x and y, the composition calculus implies that $(i \pm H_0)^{-1}W_0 \in \mathrm{Op}(S(\langle x, y, \xi, \zeta\rangle^{-2}))$, meaning that $(i\pm H_0)^{-1}W_0$ is compact. Thus $(i\pm H_0)^{-1}W$ is compact, meaning that W satisfies the assumptions of Theorem 3.2.10. Although W also satisfies the assumptions of Theorem 3.2.9, the latter cannot be used to prove $\sigma_I(H + W) = \sigma_I(H)$ when a is sufficiently large. Again it is clear that Theorem 3.2.11 does not apply, as W is not compactly supported in x. Since W is not continuous, Theorem 3.2.12 does not apply either.

Example 3. Suppose $W(x) = W \in \mathcal{C}_c^\infty(\mathbb{R})$, so that Theorem 3.2.11 applies. Then the symbol of $\Phi_0(H_0)W$ does not decay in y, meaning that Theorem 3.2.12 does not apply and that $\Phi_0(H_0)W$ is not trace-class. Thus W does not satisfy the assumptions of Theorem 3.2.9 or 3.2.10.

Example 4. Suppose $W = W(x, y) = \langle x, y\rangle^{-\delta}$ for some $0 < \delta < 1$. It is clear that W satisfies the assumptions of Theorem 3.2.12, but does not decay fast enough to meet the criteria of Theorems 3.2.9–3.2.11.

CHAPTER 4

PERIODIC SYSTEMS

This section concerns computational approximations of $\sigma_I(H,P)$. A standard method to approximate spectral decompositions of operators in $\mathbb{R}^2$ is to consider the restriction of the operator on a box $(-\pi L, \pi L)^2$ with periodic boundary conditions and analyze the limit $L \to \infty$. However, because of the structure of the domain wall with $\sigma(y)$ transitioning from σ_- to σ_+ as y crosses 0, any periodization generates another transition from σ_+ to σ_- as y crosses πL. The asymmetric transport along the x axis when y is close to 0 is compensated by an asymmetric transport along the x axis when y is close to $-\pi L \equiv \pi L$ with opposite chirality, resulting in a (globally) topologically trivial material.

Periodic systems thus no longer enjoy a non-trivial topology. This is a no-go result similar to a fermion doubling or Nelson-Ninomiya theorem [87] ensuring that any domain wall in a mass term on a torus, no matter how large, may continuously be deformed to a constant mass term. The trace in (1.0.1) therefore needs to be modified so the integral focuses on the original domain wall, which as $L \to \infty$ becomes well separated from the spurious second domain wall. While conductivities may be computed for general pseudo-differential Hamiltonians, as we do in Section 2, see also [11], we restrict our analysis of periodized Hamiltonians to differential systems and avoid complications resulting from non-local effects. We therefore consider (unperturbed) infinite-space Hamiltonians that satisfy (H1) and are differential operators of the form

$$H = M_0 D_y^m + M_m D_x^m + \sum_{j=0}^{m} a_j(y) D_x^j D_y^{m-j} + \sum_{i+j \le m-1} a_{ij}(y) D_x^i D_y^j, \tag{4.0.1}$$

where $D_x = -i\partial_x$ and $D_y = -i\partial_y$ and M_0 and M_m are constant nonsingular Hermitian matrices, while

$$\{M_0, M_m\} \begin{cases} = 0, & m \text{ is odd} \\ \geq 0, & m \text{ is even} \end{cases}, \qquad \{M_i, a_j(y)\} \begin{cases} = 0, & i+j \text{ is odd} \\ \geq 0, & i+j \text{ is even} \end{cases}, \tag{4.0.2}$$

with the second condition understood to hold for all $i \in \{0, m\}$, $j \in \{0, 1, \ldots, m\}$, and $y \in \mathbb{R}$. The $a_j(y)$ and $a_{ij}(y)$ are smooth matrix-valued functions such that H is symmetric. In particular, this means the leading-order coefficients $a_j(y)$ are all Hermitian-valued. The anti-commutation relations (4.0.2) with $\{O_1, O_2\} := O_1 O_2 + O_2 O_1$ for two operators O_1 and O_2 ensure that $H^2 = M_0^2 D_y^{2m} + M_m^2 D_x^{2m} + A + B$, where A is non-negative and B is a differential operator of order $2m-1$, so that H^2 remains a self-adjoint elliptic operator. We need the above structure in some applications to superconductors. We will finally consider perturbed operators $H_V = H + V$ where $V = V(x, y)$ is a multiplication operator with support that remains sufficiently close, in an appropriate sense, to the center of the torus.

To approximate H by an operator on $(-\pi L, \pi L)^2$, we redefine the coefficients near $y = \pi L$ so that they are smoothly connected there. The resulting periodic Hamiltonian is unitarily equivalent to an operator H_λ on $(-\pi, \pi)^2$, with $\lambda = L^{-1}$ the relevant parameter. The details of the construction of H_λ are left for section 4.1. For $\varphi \in \mathfrak{S}(0, 1; E_1, E_2)$, we define the *periodic interface conductivity* by

$$\tilde{\sigma}_I(H_\lambda) = \operatorname{Tr} iQ[H_\lambda, P]\varphi'(H_\lambda), \tag{4.0.3}$$

where $P = P(x)$ and $Q = Q(x, y) = Q_X(x) Q_Y(y)$ are smooth point-wise multiplication operators such that

$$Q_\Theta(\theta) = \begin{cases} 1, & |\theta| \leq \pi/2 \\ 0, & |\theta| \geq \pi/2 + \delta_Q \end{cases}$$

and

$$P(x) = \begin{cases} 0, & x_1 \leq x \leq x_2 \qquad -\pi < x_1 < -3\pi/4 < -\pi/2 < x_2 \\ 1, & x_3 \leq x \leq x_4 \qquad x_2 < x_3 < \pi/2 < 3\pi/4 < x_4 < \pi, \end{cases}$$

for some fixed $0 < \delta_Q < \pi/4$. As we may observe, Q is a spatial filter centered at the domain wall of interest where $P' > 0$ and vanishing in the vicinity of the unwanted domain wall where $P' < 0$.

Our main result in Section 4.1 shows that $|\tilde{\sigma}_I(H_\lambda) - \sigma_I(H)| \lesssim \lambda^p$ for any $p \geq 0$ as $\lambda \to 0$, which corresponds to an almost-exponential rate of convergence. This is based on a careful approximation of the periodic eigenfunctions by truncations of the infinite eigenfunctions corresponding to energies in the bulk spectral gap in the vicinity of domain walls and on a proof that such periodic eigenfunctions have to be negligible away from the domain walls. Estimates of the periodic eigenelements by means of min-max theorems allow us to obtain the above trace estimates.

We next prove in Section 4.2 that for a large class of perturbations V_λ with appropriate support constraints, $|\tilde{\sigma}_I(H_\lambda + V_\lambda) - \tilde{\sigma}_I(H_\lambda)| \lesssim \lambda^p$ as $\lambda \to 0$, for all $p \geq 0$. These results of approximate stability of conductivities in a periodic setting parallel the exact stability results in Euclidean space of Section 2.

Section 4.3 finally shows how the above theory applies to the models from solid state physics that were already considered in Section 2.3.

Section 4.4 presents several numerical simulations highlighting our theoretical findings. In particular, we demonstrate for several differential operators that $\tilde{\sigma}_I$ is a good numerical approximation of the infinite-space conductivity σ_I and is stable under perturbations by sufficiently localized point-wise multiplication operators.

We also confirm numerically several theoretical results obtained for a topologically non-trivial 3×3 system of water wave equations. In particular, it is known that the bulk-interface correspondence may fail for certain domain wall profiles of the un-regularized system. We confirm numerically results derived in [10] and showing that the conductivity is stable for some 3×3 perturbations V but not all. We also confirm results obtained in earlier sections that a regularized version of the water wave system does have a stable, well defined, edge conductivity equal to 2.

4.1 Periodic approximations of infinite-space problems

This section addresses approximations of a Hamiltonian in $\mathbb{R}^2$ by an operator on the 2-torus $\mathbb{T}^2$. Throughout this thesis, $\mathbb{T}$ is identified with $[-\pi, \pi)$. We construct the periodic operator H_λ introduced above and show that the periodic interface conductivity (4.0.3) is a good approximation of its infinite-space analogue (1.0.1).

Let us introduce the following Hilbert spaces

$$\mathcal{H}^j(X) := \{\Psi \in L^2(X) \otimes \mathbb{C}^n \quad | \quad \partial_\alpha \Psi \in L^2(X) \otimes \mathbb{C}^n \quad \forall\ |\alpha| \leq j\},$$

where $j \in \mathbb{N}$ and $X \in \{\mathbb{R}^d, \mathbb{T}^d\}$ with $d \in \{1, 2\}$. For $X = \mathbb{T}^d$ and a parameter $\lambda \in (0, 1]$, we define on $\mathcal{H}^j(X)$ the inner products and norms

$$\langle f, g\rangle_{\lambda,j} := \sum_{|\alpha|\leq j} \langle \lambda^{|\alpha|} D^\alpha f, \lambda^{|\alpha|} D^\alpha g\rangle, \qquad \|f\|_{\lambda,j} := \langle f, f\rangle_{\lambda,j}^{1/2},$$

with $\langle \cdot, \cdot\rangle$ the standard inner product in $L^2(\mathbb{T}^d) \otimes \mathbb{C}^n$. For $X = \mathbb{R}^d$, the corresponding inner product and norm are

$$(f, g)_j := \sum_{|\alpha|\leq j} (D^\alpha f, D^\alpha g), \qquad |||f|||_j := (f, f)_j^{1/2},$$

with $(\cdot,\cdot)$ the standard inner product in $L^2(\mathbb{R}^d)\otimes\mathbb{C}^n$. We will use the shorthand

$$\mathcal{H}(X) := \mathcal{H}^0(X), \quad \mathcal{H} := \mathcal{H}(\mathbb{R}^2), \quad \langle\cdot,\cdot\rangle_j := \langle\cdot,\cdot\rangle_{1,j}, \quad \langle\cdot,\cdot\rangle := \langle\cdot,\cdot\rangle_0, \quad (\cdot,\cdot) := (\cdot,\cdot)_0.$$

We will repeatedly need to rescale functions with λ, embed functions on $\mathbb{R}$ in the torus, and extend functions on $\mathbb{T}$ as functions on $\mathbb{R}$. We define these operations as follows. For $\lambda \in (0,1]$ and $y_1 \in \mathbb{R}$, define the unitary map $\Lambda_{\lambda,y_1} : \mathcal{H}(\mathbb{R}) \to \mathcal{H}(\mathbb{R})$ by

$$(\Lambda_{\lambda,y_1}(u))(y) := \lambda^{1/2} u(\lambda(y-y_1)+y_1), \qquad y \in \mathbb{R}.$$

Observe that $\Lambda^{-1}_{\lambda,y_1} = \Lambda_{\lambda^{-1},y_1}$.

Let $L^\infty_{c,2\pi}(\mathbb{R})$ denote the space of bounded functions $f \in L^\infty_c(\mathbb{R})$ such that $\mathrm{supp}(f) \in (\tau,\tau+2\pi)$ for $\tau\in\mathbb{R}$. We define by $f_\sharp(y) = \sum_{q\in\mathbb{Z}} f(2\pi q + y)$ their periodization (which is smooth when f is smooth) and then $\mathcal{P} : L^\infty_{c,2\pi}(\mathbb{R}) \to L^\infty(\mathbb{T})$ by

$$\mathcal{P}u(y) = u_\sharp(y) = \sum_{q\in\mathbb{Z}} u(2\pi q + y).$$

Thus, $\mathcal{P}$ is an embedding of functions on $\mathbb{R}$ with sufficiently small support to functions on $\mathbb{T}$.

We define $\tilde{\mathcal{P}}$ as the operator mapping a function in $u \in L^\infty(\mathbb{T})$ to $L^\infty_c(\mathbb{R})$ by

$$\tilde{\mathcal{P}}u(y) = \chi_{[-\pi,\pi)}(y)u((y+\pi) \bmod 2\pi - \pi)$$

with χ_I the indicatrix function of $I \subset \mathbb{R}$.

For u vector-valued, $\mathcal{P}u$ and $\tilde{\mathcal{P}}u$ are defined as above component-wise.

Construction of the periodic operator. We now construct a differential operator on the torus. We start from our original operator $H = \mathrm{Op}(\sigma)$, assumed to be a differential operator on $\mathcal{H} = L^2(\mathbb{R}^2) \otimes \mathbb{C}^n$ given by (4.0.1) and (4.0.2) such that σ satisfies (H1).

Any operator with smooth coefficients on the torus will have a transition modeling a domain wall between σ_- and σ_+ in the vicinity of $y = 0$ and another domain wall from σ_+ to σ_- in the vicinity of $y = \pi$. We construct a differential operator $H' = \mathrm{Op}(\sigma')$ with such a domain wall, i.e., such that $\sigma' = \sigma_+$ whenever $y \leq \pi - y_0$ and $\sigma' = \sigma_-$ whenever $y \geq \pi + y_0$. Assume that σ' is smooth and independent of x, and that for every $y' \in \mathbb{R}$, there exists $y \in \mathbb{R}$ such that $\sigma'(y', \xi, \zeta) = \sigma(y, \xi, \zeta)$. We may for instance choose $\sigma'(y, \xi, \zeta) = \sigma(\pi - y, \xi, \zeta)$.

The above operators are defined on $\mathbb{R}$ and need to be mapped to a torus and glued together. Define the rescaled versions $\tilde{H}_\lambda = \mathrm{Op}(\tilde{\sigma}_\lambda)$ and $\tilde{H}'_\lambda = \mathrm{Op}(\tilde{\sigma}'_\lambda)$, where $\tilde{\sigma}_\lambda(y, \xi, \zeta) := \sigma(y/\lambda, \lambda\xi, \lambda\zeta)$ and $\tilde{\sigma}'_\lambda(y, \xi, \zeta) := \sigma'(\frac{y-\pi}{\lambda} + \pi, \lambda\xi, \lambda\zeta)$. Then there exists $\lambda_0 \in (0, 1]$ such that for all $\lambda \in (0, \lambda_0]$, we can define H_λ a differential operator on $\mathcal{H}(\mathbb{T}^2) = L^2(\mathbb{T}^2) \otimes \mathbb{C}^n$ with *smooth coefficients* that are equal to those of $\tilde{H}_\lambda$ when $-\pi/2 \leq y \leq \pi/2$ and $\tilde{H}'_\lambda$ when $\pi/2 \leq y \leq 3\pi/2$ (with the equivalence $-\pi/2 \equiv 3\pi/2$ on $\mathbb{T}$). Thus we have

$$H_\lambda = \lambda^m \Big(M_0 D_y^m + M_m D_x^m + \sum_{j=0}^{m} a_{\lambda,j}(y) D_x^j D_y^{m-j} \Big) + \sum_{i+j \leq m-1} \lambda^{i+j} a_{\lambda,ij}(y) D_x^i D_y^j, \tag{4.1.1}$$

where the $a_{\lambda,j}, a_{\lambda,ij} \in \mathcal{C}_c^\infty(\mathbb{T})$ are constant whenever $\lambda y_0 \leq |y| \leq \pi - \lambda y_0$. By definition, we know that for all $j \in \{0, 1, \ldots, m\}$ and $y \in \mathbb{T}$, there exists $y' \in \mathbb{R}$ such that $a_{\lambda,j}(y) = a_j(y')$. Hence (4.0.2) holds in the periodic setting, with a_j replaced by $a_{\lambda,j}$. Moreover, for any multi-index $\alpha \in \mathbb{N}^2$, we have $\lambda^{|\alpha|}(\sum_j \left\|\partial^\alpha a_{\lambda,j}\right\|_{L^\infty} + \sum_{i,j} \left\|\partial^\alpha a_{\lambda,ij}\right\|_{L^\infty}) \leq C$ uniformly in λ.

The Hamiltonian $H - \frac{E_1+E_2}{2}$ satisfies the same assumptions as H, thus we can take $-E_1 = E_2 =: E > 0$ without loss of generality. To simplify the following calculations, we will assume that φ' is even, so we can let $\Upsilon \in \mathcal{C}_c^\infty(-1, E^2 - \delta_0)$ for some $\delta_0 > 0$, such that $\varphi'(x) = \Upsilon(x^2)$ for all $x \in \mathbb{R}$. Recall that by Corollary 2.4.4, the infinite-space conductivity

$\sigma_I(H)$ is independent of $\varphi \in \mathfrak{S}(0,1;-E,E)$.

The main result of this section is the following, where σ_I and $\tilde{\sigma}_I$ are given by (1.0.1) and (4.0.3), respectively.

Theorem 4.1.1. *For any $p > 0$, there exists a constant $C_p > 0$ such that $|\sigma_I(H) - \tilde{\sigma}_I(H_\lambda)| \leq C_p \lambda^p$ as $\lambda \to 0$.*

Hidden in Theorem 4.1.1 is the assertion that $\varphi'(H_\lambda)$ is well defined. It suffices to show that H_λ is self-adjoint [70], which we do by creating a continuous path between H_λ and a corresponding differential operator with constant coefficients. To this end, define

$$H_{\lambda,\mu} := \lambda^m \Big(M_0 D_y^m + M_m D_x^m \Big) \\ + \mu \Big(\lambda^m \sum_{j=0}^{m} a_{\lambda,j}(y) D_x^j D_y^{m-j} + \sum_{i+j \leq m-1} \lambda^{i+j} a_{\lambda,ij}(y) D_x^i D_y^j \Big)$$

for $\mu \in [0,1]$. Note that $H_{\lambda,\mu}$ is symmetric since H_λ is.

Proposition 4.1.2. *There exist positive constants C_1 and C_2 such that for all $f \in \mathcal{H}^m(\mathbb{T}^2)$,*

$$\left\| H_{\lambda,\mu} f \right\|^2 \geq C_1 \left\| f \right\|_{\lambda,m}^2 - C_2 \left\| f \right\|^2$$

uniformly in $\lambda \in (0, \lambda_0]$ and $\mu \in [0,1]$.

In the following proof, we use the Gagliardo-Nirenberg inequality on the Torus which states that for any non-negative integers i and j satisfying $i + j \leq m$,

$$\left\| \partial_x^i \partial_y^j f \right\| \leq \left\| \partial_x^m f \right\|^{\frac{i}{m}} \left\| \partial_y^m f \right\|^{\frac{j}{m}} \left\| f \right\|^{1 - \frac{i+j}{m}} \tag{4.1.2}$$

for all $f \in \mathcal{H}^m(\mathbb{T}^2)$.

Proof. From the anti-commutation properties (4.0.2), we see that $H_{\lambda,\mu}^2 = \lambda^{2m} \Big(M_0^2 D_y^{2m} +$

$M_m^2 D_x^{2m}\Big) + A_{\lambda,\mu} + B_{\lambda,\mu}$, where

$$A_{\lambda,\mu} = \lambda^{2m}\Bigg(\{M_0, M_m\}D_y^m D_x^m + \mu \sum_{j=0}^{\lfloor \frac{m}{2} \rfloor} \Big(D_x^{2j} D_y^{m-j}\{M_0, a_{\lambda,2j}\}D_y^{m-j} + D_x^{2(m-j)} D_y^j \{M_m, a_{\lambda,m-2j}\}D_y^j\Big) + \Big(\mu \sum_{j=0}^{m} a_{\lambda,j}(y) D_x^j D_y^{m-j}\Big)^2\Bigg)$$

is non-negative and

$$B_{\lambda,\mu} = \sum_{i+j \le 2m-1} \lambda^{i+j} \tilde{a}_{\lambda,\mu,ij}(y) D_x^i D_y^j$$

is of order $2m-1$, with $\lambda^{|\alpha|} \sum_{i,j} \left\|\partial^\alpha \tilde{a}_{\lambda,\mu,ij}\right\|_{L^\infty} \le C_\alpha$ uniformly in λ and μ for all $\alpha \in \mathbb{N}^2$. Using that M_0 and M_m are non-singular and Hermitian, we have

$$\left\|H_{\lambda,\mu} f\right\|^2 \ge \lambda^{2m} c(\left\|D_y^m f\right\|^2 + \|D_x^m f\|^2) + (f, B_{\lambda,\mu} f)$$

for some $c > 0$. The result then follows from (4.1.2) and the fact that $|(f, B_{\lambda,\mu} f)| \le C \|f\|_{\lambda,m} \|f\|_{\lambda,m-1}$. □

Proposition 4.1.2 implies the existence of a positive constant C such that $\|f\|_{\lambda,m} \le C \|g\|$ for all $f \in \mathcal{H}^m(\mathbb{T}^2)$ and $g \in \mathcal{H}(\mathbb{T}^2)$ satisfying $(i - H_{\lambda,\mu})f = g$ uniformly in λ and μ. Indeed, redefining the constants C_1 and C_2, we have

$$\|f\|_{\lambda,m}^2 \le C_1 \left\|H_{\lambda,\mu} f\right\|^2 + C_2 \|f\|^2 = C_1 \|g - if\|^2 + C_2 \|f\|^2 \le C^2 \|g\|^2, \tag{4.1.3}$$

where the last inequality follows from the fact that $\|f\|^2 = \Im(f, (i - H_{\lambda,\mu})f) = \Im(f, g) \le \|f\| \|g\|$. Clearly the same bound (4.1.3) holds if $i - H_{\lambda,\mu}$ is replaced by $i + H_{\lambda,\mu}$.

Proposition 4.1.3. *For all $\lambda \in (0, \lambda_0]$, H_λ is self-adjoint on $\mathcal{H}(\mathbb{T}^2)$ with domain of definition $\mathcal{H}^m(\mathbb{T}^2)$.*

Proof. By (4.1.3) and regularity of the coefficients of $H_{\lambda,\mu}$, we can choose $N \in \mathbb{N}$ sufficiently large such that $\left\|(H_{\lambda,(k+1)/N} - H_{\lambda,k/N})f\right\| \le \|g\|/2$ for all $g \in \mathcal{H}(\mathbb{T}^2)$, $f \in \mathcal{H}^m(\mathbb{T}^2)$ satisfying $(i - H_{\lambda,k/N})f = g$, and $k \in \{0, 1, \dots, N-1\}$. Since $H_{\lambda,0}$ is symmetric with constant coefficients, we know (or easily verify) that $i - H_{\lambda,0}$ is a bijection $\mathcal{H}^m(\mathbb{T}^2) \to \mathcal{H}(\mathbb{T}^2)$. Now, suppose $i - H_{\lambda,k/N}$ is a bijection $\mathcal{H}^m(\mathbb{T}^2) \to \mathcal{H}(\mathbb{T}^2)$ for some $k \in \{0, 1, \dots, N-1\}$, meaning that $\left\|(H_{\lambda,(k+1)/N} - H_{\lambda,k/N})(i - H_{\lambda,k/N})^{-1}\right\| \le 1/2$. Then

$$i - H_{\lambda,(k+1)/N} = \Big(1 - (H_{\lambda,(k+1)/N} - H_{\lambda,k/N})(i - H_{\lambda,k/N})^{-1}\Big)(i - H_{\lambda,k/N})$$

is a bijection $\mathcal{H}^m(\mathbb{T}^2) \to \mathcal{H}(\mathbb{T}^2)$, as the first factor on the above right-hand side can be inverted using the Neuman series. We conclude by induction that $i - H_{\lambda,1} = i - H_\lambda$ is a bijection $\mathcal{H}^m(\mathbb{T}^2) \to \mathcal{H}(\mathbb{T}^2)$. The same reasoning implies that $i + H_\lambda$ is a bijection $\mathcal{H}^m(\mathbb{T}^2) \to \mathcal{H}(\mathbb{T}^2)$. Since H_λ is symmetric, it follows from [70, Theorem VIII.3] that H_λ is self-adjoint with domain of definition $\mathcal{H}^m(\mathbb{T}^2)$. This completes the proof. □

For $\xi \in \mathbb{R}$, define the differential operator $\hat{H}(\xi)$ on $\mathcal{H}(\mathbb{R})$ by

$$\hat{H}(\xi) := M_0 D_y^m + M_m \xi^m + \sum_{j=0}^{m} a_j(y)\xi^j D_y^{m-j} + \sum_{i+j \le m-1} a_{ij}(y)\xi^i D_y^j.$$

Since the coefficients of H are independent of x, we have the decomposition

$$H = \mathcal{F}^{-1}_{\xi\to x} \int_{\mathbb{R}}^{\oplus} \hat{H}(\xi) d\xi \mathcal{F}_{x\to\xi},$$

with $\mathcal{F}$ the one dimensional Fourier transform in the x-variable.

For $\lambda \in (0, \lambda_0]$ and $\xi \in \mathbb{R}$, define the differential operator $\hat{H}_\lambda(\xi)$ on $\mathcal{H}(\mathbb{T})$ by

$$\hat{H}_\lambda(\xi) := \lambda^m M_0 D_y^m + M_m \xi^m + \sum_{j=0}^{m} \lambda^{m-j} a_{\lambda,j}(y)\xi^j D_y^{m-j} + \sum_{i+j \le m-1} \lambda^j a_{\lambda,ij}(y)\xi^i D_y^j. \tag{4.1.4}$$

Noting that the coefficients of H_λ are independent of x, we see that for any $\psi \in \mathcal{H}^m(\mathbb{T})$ and $\xi \in \mathbb{Z}$,

$$(\hat{H}_\lambda(\lambda\xi)\psi)(y) = e^{-i\xi x}(H_\lambda \psi_\xi)(x,y)$$

for all $(x,y) \in \mathbb{T}^2$, where $\psi_\xi \in \mathcal{H}^m(\mathbb{T}^2)$ is given by $\psi_\xi(x,y) = e^{i\xi x}\psi(y)$.

One can easily apply the logic from the proofs of Propositions 4.1.2 and 4.1.3 to obtain analogous results for $\hat{H}_\lambda(\xi)$. Namely, there exist positive constants C_1 and C_2 such that for all $f \in \mathcal{H}^m(\mathbb{T})$,

$$\left\| \hat{H}_\lambda(\xi) f \right\|^2 \geq (C_1 \xi^{2m} - C_2) \|f\|^2 + C_1 \left\| \lambda^m D_y^m f \right\|^2 \tag{4.1.5}$$

uniformly in $\lambda \in (0, \lambda_0]$ and $\xi \in \mathbb{R}$. As above, this implies that $\hat{H}_\lambda(\xi)$ is self-adjoint with domain of definition $\mathcal{H}^m(\mathbb{T})$. In addition, we obtain

Proposition 4.1.4. *The operator $\hat{H}_\lambda^2(\xi)$ is self-adjoint with domain of definition $\mathcal{H}^{2m}(\mathbb{T})$ and its spectrum consists only of eigenvalues that go to $+\infty$.*

Proof. Clearly $\hat{H}_\lambda^2(\xi)$ is symmetric. Moreover, we see that $i + \hat{H}_\lambda^2(\xi) = (\frac{1-i}{\sqrt{2}} + \hat{H}_\lambda(\xi))(\frac{-1+i}{\sqrt{2}} + \hat{H}_\lambda(\xi))$, with each factor on the right-hand side a bijection $\mathcal{H}^{k+2m}(\mathbb{T}) \to \mathcal{H}^k(\mathbb{T})$ for any $k \in \mathbb{N}$. Thus $i + \hat{H}_\lambda^2(\xi)$ is a bijection $\mathcal{H}^{2m}(\mathbb{T}) \to \mathcal{H}(\mathbb{T})$. The same holds for $i - \hat{H}_\lambda^2(\xi)$, meaning that $\hat{H}_\lambda^2(\xi)$ is self-adjoint with domain $\mathcal{H}^{2m}(\mathbb{T})$.

To prove the spectral property, we write $(1+\hat{H}_\lambda^2(\xi))^{-1} = (1+\hat{H}_\lambda^2(\xi))^{-1}(1+\hat{H}_{\lambda,0}^2(\xi))(1+\hat{H}_{\lambda,0}^2(\xi))^{-1}$ for $\hat{H}_{\lambda,0}(\xi) := M_0\lambda^m D_y^m + M_m\xi^m$. Since $\hat{H}_{\lambda,0}(\xi)$ has constant coefficients, it is clear that $(1+\hat{H}_{\lambda,0}^2(\xi))^{-1}$ is Hilbert-Schmidt. Since $(1+\hat{H}_\lambda^2(\xi))^{-1}(1+\hat{H}_{\lambda,0}^2(\xi))$ is bounded, we conclude that $(1+\hat{H}_\lambda^2(\xi))^{-1}$ is Hilbert-Schmidt, hence compact. Therefore the spectrum of $(1+\hat{H}_\lambda^2(\xi))^{-1}$ consists entirely of eigenvalues that converge to 0, meaning that the spectrum of $\hat{H}_\lambda^2(\xi)$ consists only of eigenvalues tending to $+\infty$. $\square$

We now state the following well known result characterizing the spectrum of self-adjoint operators, which can be found in, e.g., [71, 81].

Theorem 4.1.5. *Let $A : \mathcal{H}_0 \to \mathcal{H}_0$ be self-adjoint with $\mathcal{H}_0$ a separable Hilbert space, and let $E_1 \leq E_2 \leq E_3 \dots$ be the eigenvalues of A below the essential spectrum (counted with multiplicity), respectively, the infimum of the essential spectrum, once there are no more eigenvalues left. Let v_j denote the eigenfunction corresponding to E_j (when the latter is an eigenvalue), such that $\langle v_i, v_j\rangle = \delta_{ij}$ for all i and j. Then for any $\ell \in \mathbb{N}_+$ and $u \in span(v_1, v_2, \dots, v_{\ell-1})^\perp$, $\langle u, Au\rangle \geq E_\ell \|u\|^2$. Moreover, we have*

$$
\begin{aligned}
E_\ell &= \max_{\phi_1,\dots,\phi_{\ell-1}} \min\{\langle \phi, A\phi\rangle : \phi \in span(\phi_1, \dots, \phi_{\ell-1})^\perp,\ \|\phi\| = 1\} \\
&= \min_{\phi_1,\dots,\phi_\ell} \max\{\langle \phi, A\phi\rangle : \phi \in span(\phi_1, \dots, \phi_\ell),\ \|\phi\| = 1\}.
\end{aligned}
$$

We now gather useful properties of the infinite-space operator $\hat{H}(\xi)$ and its spectrum.

Proposition 4.1.6. *Take $H = \mathrm{Op}(\sigma)$ as above, and fix $\delta > 0$. Then for each $\xi \in \mathbb{R}$, $\hat{H}(\xi)$ and $\hat{H}^2(\xi)$ are self-adjoint with respective domains of definition $\mathcal{H}^m(\mathbb{R})$ and $\mathcal{H}^{2m}(\mathbb{R})$. The spectrum of $\hat{H}^2(\xi)$ in the interval $[0, E^2 - \delta)$ consists of a finite number of eigenvalues, each with finite multiplicity. These eigenvalues and corresponding eigenfunctions can be chosen so that they are analytic in ξ. Moreover, the rank of $\hat{H}^2(\xi)$ in $[0, E^2 - \delta)$ is uniformly bounded in $\xi \in \mathbb{R}$ and vanishes whenever $|\xi|$ is sufficiently large.*

Proof. Fix $\xi \in \mathbb{R}$. Since $\hat{H}(\xi) = \mathrm{Op}(\sigma_\xi)$ with $\sigma_\xi \in S^m_{1,0}$ elliptic, it follows from [20, 56] that $\hat{H}(\xi)$ is self-adjoint with domain of definition $\mathcal{H}^m(\mathbb{R})$. We know that $\hat{H}^2(\xi) = \mathrm{Op}(\tau_\xi)$, where $\tau_\xi(y,\zeta) = (\sigma \sharp \sigma)(y, \xi, \zeta)$. Applying the same argument to the elliptic symbol $\tau_\xi \in S^{2m}_{1,0}$, wee see that $\hat{H}^2(\xi)$ is self-adjoint with domain of definition $\mathcal{H}^{2m}(\mathbb{R})$. Define $\sigma_{\pm,\xi}(\zeta) := \sigma_\pm(\xi, \zeta)$ and $\tau_{\pm,\xi} := \sigma^2_{\pm,\xi}$, and observe that $\tau_\xi = \tau_{+,\xi}$ whenever $y \geq y_0$, and $\tau_\xi = \tau_{-,\xi}$ whenever

$y \le -y_0$. Since the $\tau_{\pm,\xi}$ are independent of y,

$$T_{\pm,\xi} := \mathrm{Op}(\tau_{\pm,\xi}) = (\mathrm{Op}(\sigma_{\pm,\xi}))^2 \ge 0.$$

Let $\chi \in \mathfrak{S}(0, \pi/2, -1, 1)$, and define $\chi_\varepsilon(y) := \chi(\varepsilon y)$ and

$$\mathrm{Op}(\tau_{\varepsilon,\xi}) = T_{\varepsilon,\xi} := \sin(\chi_\varepsilon(y))T_{+,\xi}\sin(\chi_\varepsilon(y)) + \cos(\chi_\varepsilon(y))T_{-,\xi}\cos(\chi_\varepsilon(y))$$

for $\varepsilon \in (0, 1]$. We see that $\tau_{\varepsilon,\xi} = \sin^2(\chi_\varepsilon(y))\tau_{+,\xi} + \cos^2(\chi_\varepsilon(y))\tau_{-,\xi} + \varepsilon r_{\varepsilon,\xi}$, with $r_{\varepsilon,\xi} \in S(\langle\zeta\rangle^{2m})$ uniformly in ε, and $\tau_{\pm,\xi} \ge \max\{E^2, c\langle\zeta\rangle^{2m}\}$. It follows that

$$\tau_{\varepsilon,\xi} \ge \max\{E^2, c\langle\zeta\rangle^{2m}\} - c'\varepsilon\langle\zeta\rangle^{2m}$$

for some positive constant c', hence $\tau_{\varepsilon,\xi} \ge E^2 - \delta/4$ for ε sufficiently small. Using the fact that $T_{\varepsilon,\xi} \ge 0$, we apply Lemma 4.1.7 below (with a unitary transformation) to conclude that $T_{\varepsilon,\xi}$ has no spectrum in the interval $(-\infty, E^2 - \delta/2)$ for ε sufficiently small.

We now observe that

$$\begin{aligned}(i - T_{\varepsilon,\xi})^{-1} - (i - \hat{H}^2(\xi))^{-1} &= \\ &(i - T_{\varepsilon,\xi})^{-1}(\hat{H}^2(\xi) - T_{\varepsilon,\xi})(i - \hat{H}^2(\xi))^{-1} \in \mathrm{Op}(S(\langle y\rangle^{-\infty}\langle\zeta\rangle^{-2m})),\end{aligned}$$

as $\tau_\xi - \tau_{\varepsilon,\xi} \in S(\langle y\rangle^{-\infty}\langle\zeta\rangle^{2m})$ and both resolvents have symbol in $S(\langle\zeta\rangle^{-2m})$. Since $\langle\zeta\rangle^{-2m} \in L^2(\mathbb{R})$, it follows that $(i - T_{\varepsilon,\xi})^{-1} - (i - \hat{H}^2(\xi))^{-1}$ is Hilbert-Schmidt, hence compact. By [81, Theorem 6.18], we conclude that the essential spectra of $T_{\varepsilon,\xi}$ and $\hat{H}^2(\xi)$ are the same, meaning that the spectrum of $\hat{H}^2(\xi)$ in $[0, E^2 - \delta/2)$ consists of eigenvalues, each with finite multiplicity. The number of these eigenvalues must be finite, as we can verify from the proof of Proposition 2.1.10 that $\Phi_0(\hat{H}^2(\xi))$ is trace-class for all $\Phi_0 \in \mathcal{C}_c^\infty(-1, E^2)$.

Fix $\xi \in \mathbb{R}$. Let $\psi \in \mathcal{C}_c^\infty(\mathbb{R}) \otimes \mathbb{C}^n$ such that $|||\psi||| = 1$. Define $\tilde{\psi} := \Lambda_{\lambda_1,0}^{-1}\psi$, where

$\lambda_1 \in (0, \lambda_0]$ is sufficiently small so that $\mathrm{supp}(\tilde{\psi}) \subset (-\pi/2, \pi/2)$. Then by (4.1.5),

$$\left|\left|\left|\hat{H}(\xi)\psi\right|\right|\right| = \left\|\hat{H}_{\lambda_1}(\xi)\mathcal{P}\tilde{\psi}\right\| \geq C_1\xi^m - C_2.$$

Since $\mathcal{C}_c^\infty(\mathbb{R})$ is dense in $\mathcal{H}^m(\mathbb{R})$ with respect to the $\mathcal{H}^m$-norm, we have proved that $\hat{H}^2(\xi)$ has no spectrum in $[0, E^2)$ whenever $|\xi|$ is sufficiently large.

Let $\nu_1(\xi) \leq \nu_2(\xi) \leq \cdots \leq \nu_{\tilde{N}(\xi)}(\xi)$ denote the eigenvalues of $\hat{H}(\xi)$ below $E^2 - \delta/2$. We showed above that $\tilde{N}(\xi)$ is finite for all $\xi \in \mathbb{R}$. Let $N(\xi)$ be the number of eigenvalues of $\hat{H}^2(\xi)$ in $[0, E^2 - \delta)$. To show that $N(\xi)$ is bounded uniformly in ξ, we will first prove that the eigenvalues are uniformly equicontinuous in ξ. By "uniformly equicontinuous", we mean that for all $\varepsilon > 0$, there exists $\eta > 0$ such that for any $|\xi_1 - \xi_2| < \eta$ and any j satisfying $j \leq \tilde{N}(\xi_1)$, it follows that $|\nu_j(\xi_2) - \nu_j(\xi_1)| < \varepsilon$.

Fix $C_0 > 0$. Let $\bar{\xi} > 0$ such that $\hat{H}^2(\xi)$ has no spectrum in $[0, E^2 - \delta/2)$ whenever $|\xi| > \bar{\xi}$. Since $\hat{H}^2(\xi + \rho) - \hat{H}^2(\xi)$ is a differential operator of order $2m - 1$ with coefficients bounded by $C|\rho|$, the Gagliardo-Nirenberg inequality (4.1.2) on $\mathbb{R}^2$ implies that

$$|(u, (\hat{H}^2(\xi + \rho) - \hat{H}^2(\xi))u)| \leq C|\rho| \, |||u|||_m^{\frac{2m-1}{m}} \, |||u|||^{\frac{1}{m}} \leq CC_0^{\frac{2m-1}{m}} |\rho| \, |||u|||^2 \tag{4.1.6}$$

uniformly in $\rho \in [-1, 1]$ and $\xi \in [-\bar{\xi}, \bar{\xi}]$, for all $u \in \mathcal{H}^m(\mathbb{R})$ satisfying $|||u|||_m \leq C_0 \, |||u|||$. By ellipticity of $\hat{H}(\xi)$, we can choose C_0 sufficiently large so that $\left|\left|\left|\hat{H}(\xi)u\right|\right|\right| \geq E \, |||u|||$ whenever $|||u|||_m > C_0 \, |||u|||$ and $\xi \in \mathbb{R}$. Hence given any ℓ-dimensional subspace $S_\ell \subset \mathcal{H}^m(\mathbb{R})$, the bound (4.1.6) holds uniformly in $u \in S_\ell$ and $\xi \in [-\bar{\xi}, \bar{\xi}]$ satisfying $\left|\left|\left|\hat{H}(\xi)u\right|\right|\right| < E \, |||u|||$. It follows that

$$\left| \max_{u \in S_\ell, |||u|||=1} (u, \hat{H}^2(\xi + \rho)u) - \max_{u \in S_\ell, |||u|||=1} (u, \hat{H}^2(\xi)u) \right| \leq CC_0^{\frac{2m-1}{2m}} |\rho|; \qquad \rho \in [-1, 1]$$

uniformly in $\xi \in [-\bar{\xi}, \bar{\xi}]$ satisfying $\max_{u \in S_\ell, |||u|||=1} \left|\left|\left|\hat{H}(\xi)u\right|\right|\right| < E$. Therefore by Theorem

4.1.5,

$$|\nu_\ell(\xi+\rho)-\nu_\ell(\xi)| = \left|\min_{S_\ell}\max_{u\in S_\ell,\|\|u\|\|=1}(u,\hat{H}^2(\xi+\rho)u) - \min_{S_\ell}\max_{u\in S_\ell,\|\|u\|\|=1}(u,\hat{H}^2(\xi)u)\right|$$
$$\le CC_0^{\frac{2m-1}{2m}}|\rho|$$

uniformly in $\rho\in[-1,1]$ and $\ell \le \tilde{N}(\xi)$. Thus we have proven uniform equicontinuity of the eigenvalues.

Suppose by contradiction that $N(\xi)$ is not bounded uniformly in ξ. Since $N(\xi)$ vanishes outside $[-\bar{\xi},\bar{\xi}]$, there exists a sequence $(\xi_k)\subset[-\bar{\xi},\bar{\xi}]$ and a number $\xi_*\in[-\bar{\xi},\bar{\xi}]$ such that $\xi_k\to\xi_*$ and $N(\xi_k)\to\infty$ as $k\to\infty$. Uniform equicontinuity of the eigenvalues implies that for all k sufficiently large, all eigenvalues ν_j satisfying $\nu_j(\xi_k) < E^2-\delta$ must also satisfy $\nu_j(\xi_*) < E^2-\delta/2$. This implies

$$\tilde{N}(\xi_*) \ge N(\xi_k) \to \infty,$$

which is a contradiction since we already proved that $\tilde{N}(\xi_*)$ must be finite.

It remains to show that the eigenvalues and eigenfunctions can be chosen analytic in ξ when they lie in $[0,E^2-\delta)$. We have shown that there exists $\tilde{N}_0<\infty$ such that $\tilde{N}(\xi)\le\tilde{N}_0$ for all $\xi\in\mathbb{R}$. Thus for all ξ such that $\nu_1(\xi)<E^2-\delta$, there exists $k(\xi)\in\{1,2,\dots,\tilde{N}_0\}$ such that $\nu_{k(\xi)+1}(\xi)\ge E^2-\delta$ and $\nu_{k(\xi)+1}(\xi)-\nu_{k(\xi)}(\xi)\ge\frac{\delta}{2\tilde{N}_0}$. Uniform equicontinuity implies that there exists $\eta>0$ such that $\nu_{k(\xi)+1}(\hat{\xi})-\nu_{k(\xi)}(\hat{\xi})\ge\frac{\delta}{4\tilde{N}_0}$ whenever $|\hat{\xi}-\xi|<\eta$. Now write $[-\bar{\xi},\bar{\xi}]\subset\cup_j B_j$, where $\{B_j\}$ is a finite collection of overlapping open intervals ($B_j\cap B_{j+1}\ne\emptyset$) of length 2η. Let ξ_j be the midpoint of B_j. Then for every j, we can apply [58, Theorems VII.1.7 and VII.1.8] to the finite system of eigenvalues $\nu_1(\xi),\nu_2(\xi),\dots,\nu_{k(\xi_j)}(\xi)$ and corresponding eigenfunctions to conclude that they can be chosen analytic in $\xi\in B_j$. Since the B_j form an open cover of $[-\bar{\xi},\bar{\xi}]$, this proves that all eigenvalues (and corresponding eigenfunctions) in the energy interval $[0,E^2-\delta)$ can be chosen analytic in ξ. This completes the result. ☐

Lemma 4.1.7. *Suppose $A_h = \mathrm{Op}_h(a)$ is non-negative for all $h \in (0,1]$, where $a \in S^m_{1,0}$ is Hermitian-valued and elliptic. Then for any constant $c \geq 0$ satisfying $a_{\min} \geq c$, there exist constants $\beta > 0$ and $0 < h_0 \leq 1$ such that $\langle \psi, A_h\psi\rangle \geq c - \beta h$ for all $\|\psi\| = 1$ and $h \in (0, h_0]$.*

Proof. We know that A_h is self-adjoint by our assumptions on a. Since $A_h \geq 0$, it follows that $(1 + A_h)^{-1} = \mathrm{Op}_h(r_h)$, where $S(1) \ni r_h = (1 + a)^{-1} + O(h)$. By the semi-classical sharp Gårding inequality [34, Theorem 7.12], there exist constants $\beta_0 > 0$ and $0 < h_0 \leq 1$ such that

$$0 < \langle \phi, (1 + A_h)^{-1}\phi\rangle \leq \Big((1 + c)^{-1} + \beta_0 h\Big) \|\phi\|^2 \tag{4.1.7}$$

for all nonzero $\phi \in \mathcal{H}$ and $h \in (0, h_0]$. Let $\psi \in \mathcal{D}(A_h)$ such that $\|\psi\| = 1$, and define $\phi = (1 + A_h)^{1/2}\psi$. Then

$$\langle \psi, (1 + A_h)\psi\rangle = \|\phi\|^2 = \frac{\|\phi\|^2}{\|\psi\|^2} = \frac{\|\phi\|^2}{\langle \phi, (1 + A_h)^{-1}\phi\rangle} \geq 1 + c - \beta h, \qquad h \in (0, h_0]$$

for some fixed constant β. This completes the proof. ☐

Spectral approximations. Recall that $H' = \mathrm{Op}(\sigma')$, where for every $y' \in \mathbb{R}$, there exists $y \in \mathbb{R}$ such that $\sigma'(y', \xi, \zeta) = \sigma(y, \xi, \zeta)$. Since σ satisfies (H1), it follows that σ' is elliptic: $|\sigma'_{\min}| \geq c\langle \xi, \zeta\rangle^m - 1$. Hence the fact that $\sigma' = \sigma_+$ whenever $y \leq \pi - y_0$ and $\sigma' = \sigma_-$ whenever $y \geq \pi + y_0$ implies that σ' also satisfies (H1), with the roles of σ_+ and σ_- reversed. We conclude that Proposition 4.1.6 still holds if H is replaced by H', where we would instead define $\tilde{\psi} := \Lambda^{-1}_{\lambda_1,\pi}\psi$ in the third paragraph of the proof.

The approximation result of Theorem 4.1.1 requires a detailed analysis of the spectrum of H_λ constructed in (4.1.1), which it inherits from that of the operators H and H'. For $\xi \in \mathbb{R}$, let $\mu_1(\xi) \leq \mu_2(\xi) \leq \mu_3(\xi) \ldots$ denote the *combined* eigenvalues of $\hat{H}^2(\xi)$ and $\hat{H}'^2(\xi)$

below $\Sigma_{\text{ess}}(\hat{H}^2(\xi)) \cup \Sigma_{\text{ess}}(\hat{H}'^2(\xi))$, respectively, the infimum of $\Sigma_{\text{ess}}(\hat{H}^2(\xi)) \cup \Sigma_{\text{ess}}(\hat{H}'^2(\xi))$, once there are no more eigenvalues left. Let R_ξ (resp. R'_ξ) be the set consisting of the indices j for which $\mu_j(\xi)$ is an eigenvalue of $\hat{H}^2(\xi)$ (resp. $\hat{H}'^2(\xi)$). Thus R_ξ and R'_ξ form a partition of the indices below $\Sigma_{\text{ess}}(\hat{H}^2(\xi)) \cup \Sigma_{\text{ess}}(\hat{H}'^2(\xi))$. When $\mu_j(\xi) \in R_\xi \cup R'_\xi$, we denote the corresponding normalized eigenfunction by $\psi_{j,\xi}(y)$. We choose the eigenfunctions so that $(\psi_{i,\xi}, \psi_{j,\xi}) = \delta_{ij}$ whenever $i, j \in R_\xi$ or $i, j \in R'_\xi$.

Let $\tilde{s}(\xi)$ be the total number of eigenvalues of $\hat{H}^2$ and $\hat{H}'^2$ lying in $[0, E^2 - \frac{\delta_0}{2})$. By Proposition 4.1.6 (and the above paragraphs), we know that $\tilde{s}(\xi)$ is indeed finite and that the eigenvalues $\mu_1(\xi) \dots \mu_{\tilde{s}(\xi)}(\xi)$ make up the entire spectrum of $\hat{H}^2(\xi)$ and $\hat{H}'^2(\xi)$ in $[0, E^2 - \frac{\delta_0}{2})$. Moreover, there exists $s_0 \in \mathbb{N}$ such that $\tilde{s}(\xi) \le s_0$ for all $\xi \in \mathbb{R}$, and there exists a compact interval $I \subset \mathbb{R}$ such that $\tilde{s}(\xi) = 0$ for all $\xi \notin I$.

Let $\mu_{\lambda,1}(\xi) \le \mu_{\lambda,2}(\xi) \le \mu_{\lambda,3}(\xi) \dots$ denote the eigenvalues of the operator $\hat{H}^2_\lambda(\xi)$ defined on the torus, which we know are well defined and go to infinity by Proposition 4.1.4. Let $\theta_{\lambda,1,\xi}, \theta_{\lambda,2,\xi}, \theta_{\lambda,3,\xi}, \dots$ be the corresponding (orthonormalized) eigenfunctions.

We now prove a result of (collective) exponential decay of the eigenfunctions of an operator with constant coefficients outside a bounded interval. This verifies that the low-energy eigenfunctions are localized to the vicinity of the domain walls, in both the periodic and infinite-space settings.

Proposition 4.1.8. *For any $\alpha \in \mathbb{N}$, there are positive constants C and r such that*

$$|\partial_y^\alpha \psi_{j,\xi}|(y) \le Ce^{-r|y|}$$

uniformly in $j \in \{1, 2, \dots, \tilde{s}(\xi)\}$ and $\xi \in I$. Similarly, given any closed interval $T \subset \mathbb{T}$ not containing 0 or π, $\left\|\lambda^\alpha \partial_y^\alpha \theta_{\lambda,j,\xi}\right\|_T \le Ce^{-r/\lambda}$ uniformly in j and ξ satisfying $\mu_{\lambda,j}(\xi) < E^2 - \delta_0/2$.

Here and below, we use the shorthand $\|\cdot\|_T := \|\cdot\|_{L^2(T)\otimes\mathbb{C}^n}$ if $T \subset \mathbb{T}$.

Proof. We first prove the claim regarding the infinite-space eigenfunctions and assume $y > 0$ for concreteness. Restricted to the region $y > y_0$, we have $\hat{H}(\xi) = \mathrm{Op}(\sigma_{+,\xi}(\zeta))$, where $\sigma_{+,\xi}(\zeta) = \sigma_+(\xi, \zeta)$. Our spectral gap assumption in (H1) is that $\sigma_+^2(\xi, \zeta)$ does not have eigenvalues inside $[0, E^2)$ while here by construction, $\mu_j \in [0, E_0^2]$ with $E_0 := \sqrt{E^2 - \frac{\delta_0}{2}} < E$. By construction of $\psi_{j,\xi}$, the statement thus follows if we can prove the bound for any solution ψ of

$$(\sigma_{+,\xi}^2(D_y) - \mu)\psi(y) = 0, \qquad y > y_0 \tag{4.1.8}$$

for an eigenvalue $\mu \in [0, E_0^2]$. We replace the above system by the first-order system

$$\frac{d}{dy} u = Au$$

for $A = A_\xi$ a $N \times N$ matrix with $N = 2mn$ and $u = (\psi, \psi', \dots, \psi^{(2m-1)})^t$. We then write $A = PJP^{-1}$ with J in Jordan form and $u = Pv$. Solving $Jv = \frac{d}{dy}v$, we see that each eigenvalue ν of J must correspond to an eigenfunction of the form $v = e^{\nu y} v_0$ so that $u = e^{\nu y} P v_0$. This means that for every such ν, there exists a solution ψ of (4.1.8) that is of the form $\psi(y) = e^{\nu y} \bar{\psi}_0$, where $\bar{\psi}_0 \in \mathbb{C}^n$ is independent of y. Since $\psi \neq 0$ by definition, this shows that

$$\det(\sigma_{+,\xi}^2(-i\nu) - \mu) = 0; \tag{4.1.9}$$

that is, $\sigma_{+,\xi}^2(-i\nu)$ must have an eigenvalue that is equal to μ. We will now show that ν must be bounded away from the imaginary axis, uniformly in all variables. First, observe that since $\sigma_{+,\xi}(\zeta)$ is bounded above by $C\langle \xi, \zeta \rangle^m$ and elliptic in ζ, there exist positive constants ν_1 and δ_1 such that whenever $|\Im\nu| > \nu_1$ and $|\Re\nu| < \delta_1$, all eigenvalues of $\sigma_{+,\xi}(-i\nu)$ lie outside $(-E, E)$. Since $\sigma_{+,\xi}(\zeta)$ is continuous in ζ and $\sigma_{+,\xi}(-i\nu)$ does not have spectrum in

$(-E, E)$ when $\Re\nu = 0$, there exists $\delta_2 > 0$ such that whenever $|\Im\nu| \leq \nu_1$ and $|\Re\nu| < \delta_2$, all eigenvalues of $\sigma_{+,\xi}(-i\nu)$ lie outside $[-E_0, E_0]$. Thus, taking $\tilde{\delta} := \min\{\delta_1, \delta_2\}$, we have shown that all ν satisfying (4.1.9) must also satisfy $|\Re\nu| \geq \tilde{\delta}$.

It is clear that $\tilde{\delta} = \tilde{\delta}(\xi, \mu)$ is continuous in both variables. Since $\sigma_{+,\xi}(\zeta)$ is bounded above by $C\langle\xi, \zeta\rangle^m$ and elliptic in ξ, there exist positive constants ξ_0 and δ_0 such that for all $|\xi| \geq \xi_0$, any ν solving (4.1.9) must also satisfy $|\Re\nu| \geq \delta_0$. Thus, setting $K := [-\xi_0, \xi_0] \times [-E_0, E_0]$ and $\delta := \min\{\delta_0, \min_{(\xi,\mu)\in K} \tilde{\delta}(\xi, \mu)\} > 0$, we have shown that all solutions ν of (4.1.9) satisfy $|\Re\nu| \geq \delta > 0$ uniformly in $\xi \in \mathbb{R}$ and $\mu \in [0, E_0^2]$.

Note that every solution ψ of (4.1.8) is a finite linear combination of terms of the form $y^k e^{\nu y} \bar{\psi}_k$, with ν satisfying (4.1.9). Since ψ is square integrable in y (and thus cannot be exponentially increasing), this shows that ψ and all of its derivatives are exponentially decreasing as $y \to \infty$, uniformly in ξ and μ. Thus we have proven the desired decay property for eigenfunctions of $\hat{H}(\xi)$ as $y \to \infty$. The argument for exponential decay as $y \to -\infty$ is identical, as is the proof for eigenfunctions of $\hat{H}'(\xi)$.

The same ideas are used for the periodic eigenfunctions, only now we must handle the λ-dependence. By definition of T, there exists a closed interval $T_1 \subset \mathbb{T}$, also not containing 0 or π, such that $T \subset T_1^\circ$. Suppose that $T_1 \subset (0, \pi)$ for concreteness. The defining equation for the eigenfunctions $\theta_{\lambda,j,\xi}$ in T_1 is

$$\sigma_+^2(\xi, \lambda D_y)\theta_{\lambda,j,\xi}(y) = \mu_{\lambda,j}(\xi)\theta_{\lambda,j,\xi}(y).$$

This is equivalent to solving an equation of the form

$$(\sigma_+^2(D_y) - \mu)f(y) = 0, \qquad f(y) = \theta_\lambda(\lambda y), \tag{4.1.10}$$

where $y \in T_{\lambda,1} := \lambda^{-1}T_1$ and $0 \leq \mu \leq E_0^2 < E^2$. The differential equation in (4.1.10) is identical to (4.1.8), with f replacing ψ. Hence $\theta_\lambda(y) = f(y/\lambda)$ is exponentially increasing or decreasing in T_1 with a rate that is proportional to λ^{-1}. Since $\theta_\lambda(y)$ has bounded L^2-norm on T_1, its L^2-norm on T is bounded by $Ce^{-r/\lambda}$ for $r > 0$. Derivatives of θ_λ also satisfy such an estimate. This completes the proof. □

What remains before proving Theorem 4.1.1 is to show that the combined spectrum (including eigenspaces) of the infinite-space Hamiltonians is a good approximation of the spectrum of the periodic Hamiltonian. We will truncate the infinite-space eigenfunctions $\psi_{j,\xi}$ so that they have compact support and can be embedded in the torus. Due to the rapid decay (in y) of these eigenfunctions and their derivatives, the truncated versions *almost* solve the eigenproblem, admitting a small residual term that goes to zero with λ. The fact that the eigenvalues for the periodic problem are themselves well approximated is the statement of Proposition 4.1.10, and follows from Lemma 4.1.9 and Theorem 4.1.5. Once the error in eigenvalues is controlled, we use Lemma 4.1.12 to show that the periodic eigenfunctions are well approximated by their infinite-space analogues, which will allow us to directly bound the error $|\tilde{\sigma}_I(H_\lambda) - \sigma_I(H)|$.

For the following results, $\xi \in \mathbb{R}$ is assumed to be arbitrary and is dropped from the notation for brevity. It will be clear that the below estimates are all uniform in ξ, given the uniform bounds from Proposition 4.1.8.

Eigenvalue approximation. Let s be the total number of eigenvalues of $\hat{H}^2$ and $\hat{H}'^2$ lying in $[0, E^2 - \delta_0)$. For $\ell \in \{0, 1, \dots, s\}$, define $\tilde{R}_\ell := \{1, 2, \dots, \ell\} \cap R$ and $\tilde{R}'_\ell := \{1, 2, \dots, \ell\} \cap R'$. [1] We will need to approximate the eigenfunctions of the infinite-space Hamiltonian by functions that live on the torus. Let $\hat{\chi}_0 \in \mathcal{C}_c^\infty(-\pi/4, \pi/4)$ such that $0 \le \hat{\chi}_0 \le 1$ on $\mathbb{R}$ and $\hat{\chi}_0 = 1$ in $[-\pi/8, \pi/8]$. Similarly, let $\hat{\chi}_\pi \in \mathcal{C}_c^\infty(\pi - \pi/4, \pi + \pi/4)$ such that $0 \le \hat{\chi}_\pi \le 1$ on $\mathbb{R}$ and $\hat{\chi}_\pi = 1$ in $[\pi - \pi/8, \pi + \pi/8]$. Define $\psi^0_{\lambda,j} := \hat{\chi}_{t_j} \Lambda^{-1}_{\lambda,t_j} \psi_j$, where $t_j = 0$ if $j \in R$ and

1. The sets $R = R_\xi$ and $R' = R'_\xi$ are defined between Propositions 4.1.6 and 4.1.8.

$t_j = \pi$ if $j \in R'$. Set $\psi_{\lambda,1} := N_{\lambda,1}\psi^0_{\lambda,1}$, and for all $j > 1$ define

$$\psi_{\lambda,j} = N_{\lambda,j}(\psi^0_{\lambda,j} - \sum_{i=1}^{j-1}\langle\psi_{\lambda,i}, \psi^0_{\lambda,j}\rangle\psi_{\lambda,i}),$$

with $N_{\lambda,j} > 0$ such that $\left\|\psi_{\lambda,j}\right\| = 1$. Thus the $\psi_{\lambda,j}$ form an orthonormal set of functions on $\mathbb{R}^2$. Let $\tilde{\psi}_{\lambda,j} := \mathcal{P}\psi_{\lambda,j}$, which is well defined since the support of each $\psi_{\lambda,j}$ is contained in an interval of length $\pi/2$.

In words, what we have done is embed the infinite-space eigenfunctions on the torus by rescaling in λ as necessary, truncating them to have compact support and orthonormalizing at the end. By the rapid decay of the $\psi_{j,\xi}$ (Proposition 4.1.8), the error we get from truncating and orthonormalizing goes to zero exponentially in λ. Namely, we have that for any $\alpha \in \mathbb{N}$, there exist positive constants C and r such that

$$\left|\!\left|\!\left|\lambda^{|\alpha|}\partial^\alpha_y(\psi_{\lambda,j} - \Lambda^{-1}_{\lambda,t_j}\psi_j)\right|\!\right|\!\right| \le Ce^{-r/\lambda} \tag{4.1.11}$$

uniformly in $\lambda \in (0, \lambda_0]$ for all $j \in \{1, 2, \ldots, s\}$.

Lemma 4.1.9. *There exist positive constants C and r such that for all $\lambda \in (0, \lambda_0], \ell \in \{0, 1, \ldots, s\}$, and $u_0 \in (span\{\tilde{\psi}_{\lambda,j}\}^{\ell}_{j=1})^\perp$ such that* $\operatorname{supp}(u_0) \subset (-\frac{3\pi}{4}, \frac{3\pi}{4})$ *or* $\operatorname{supp}(u_0) \subset (\frac{\pi}{4}, \frac{7\pi}{4})$,

$$\langle u_0, \hat{H}^2_\lambda u_0\rangle \ge \left(\min\{\mu_{\ell+1}, E^2 + 1\} - Ce^{-r/\lambda}\right)\|u_0\|^2 . \tag{4.1.12}$$

Proof. Suppose $\operatorname{supp}(u_0) \subset (-\frac{3\pi}{4}, \frac{3\pi}{4})$ for concreteness and $\|u_0\| = 1$ without loss of generality. Then for $u := \Lambda_{\lambda,0}\tilde{\mathcal{P}}u_0$, we have $\langle u_0, \hat{H}^2_\lambda u_0\rangle = (u, \hat{H}^2 u)$. Define $\tilde{u} := u - \sum_{j\in\tilde{R}_\ell}(\psi_j, u)\psi_j$, so that $(\psi_j, \tilde{u}) = 0$ for all $j \in R_\ell$, and hence

$$(\tilde{u}, \hat{H}^2\tilde{u}) \ge |\!|\!|\tilde{u}|\!|\!|^2 \min\{\mu_j : j \in (R \cup \{s_0 + 1\}) \cap \{\ell + 1, \ell + 2, \ldots, s_0 + 1\}\} \ge \mu_{\ell+1} |\!|\!|\tilde{u}|\!|\!|^2$$

by Theorem 4.1.5. Since $|||\tilde{u}|||^2 = 1 - \sum_{j\in\tilde{R}_\ell} |(\psi_j, u)|^2$, it follows that

$$(u, \hat{H}^2 u) = (\tilde{u}, \hat{H}^2 \tilde{u}) + \sum_{j\in\tilde{R}_\ell} \mu_j |(\psi_j, u)|^2 \geq \mu_{\ell+1} - \sum_{j\in\tilde{R}_\ell} (\mu_{\ell+1} - \mu_j)|(\psi_j, u)|^2.$$

Using that $(\Lambda_{\lambda,0}\psi_{\lambda,j}, u) = 0$, we see by (4.1.11) that

$$|(\psi_j, u)| = |(\Lambda_{\lambda,0}\psi_{\lambda,j} - \psi_j, u)| \leq |||\Lambda_{\lambda,0}\psi_{\lambda,j} - \psi_j||| \leq Ce^{-r/\lambda}$$

for all $j \in \tilde{R}_\ell$. We conclude that

$$(u, \hat{H}^2 u) \geq \mu_{\ell+1}(1 - Ce^{-r/\lambda}) \geq \min\{\mu_{\ell+1}, E^2 + 1\} - Ce^{-r/\lambda},$$

and the result is complete. □

We will now show that the eigenvalues for the periodic problem are well approximated by those for the infinite-space problem. The lower bounds for the $\mu_{\lambda,j}(\xi)$ will be obtained using Theorem 4.1.5 and Lemma 4.1.9.

Proposition 4.1.10. *There exist positive constants C and r such that*

$$\mu_\ell - Ce^{-r/\lambda} \leq \mu_{\lambda,\ell} \leq \mu_\ell + Ce^{-r/\lambda}$$

uniformly in $\lambda \in (0, \lambda_0]$ for all $\ell \in \{1, 2, \ldots, s\}$. Moreover, $\mu_{\lambda,s+1} \notin \mathrm{supp}(\Upsilon)$ for all λ sufficiently small.

Proof. We recall that $\varphi'(x) = \Upsilon(x^2)$. We first prove the upper bound. Fix $\lambda \in (0, \lambda_0]$ and $\ell \in \{1, \ldots, s\}$. Let $u = \sum_{j=1}^{\ell} a_j \tilde{\psi}_{\lambda,j}$ with the $a_j \in \mathbb{C}$ such that $\sum_{j=1}^{\ell} |a_j|^2 = 1$. Then

$$\langle u, \hat{H}_\lambda^2 u\rangle = \sum_{j=1}^{\ell} a_j \langle u, \hat{H}_\lambda^2 \tilde{\psi}_{\lambda,j}\rangle = \sum_{j=1}^{\ell} |a_j|^2 \mu_j + \sum_{j=1}^{\ell} a_j \langle u, (\hat{H}_\lambda^2 - \mu_j)\tilde{\psi}_{\lambda,j}\rangle,$$

with the first term on the right-hand side bounded above by μ_ℓ. To control the second term, observe that

$$\left\|(\hat{H}_\lambda^2 - \mu_j)\tilde{\psi}_{\lambda,j}\right\| = \left|\left|\left|(A_j - \mu_j)\Lambda_{\lambda,t_j}\psi_{\lambda,j}\right|\right|\right|,$$

with $(A_j, t_j) = (\hat{H}^2, 0)$ if $j \in R$ and $(A_j, t_j) = (\hat{H}'^2, \pi)$ if $j \in R'$. Using that $(A_j - \mu_j)\psi_j = 0$, we conclude that

$$\langle u, \hat{H}_\lambda^2 u\rangle \leq \mu_\ell + \sum_{j=1}^{\ell} \left|\left|\left|(A_j - \mu_j)(\Lambda_{\lambda,t_j}\psi_{\lambda,j} - \psi_j)\right|\right|\right| \leq \mu_\ell + Ce^{-r/\lambda},$$

where the last inequality follows from (4.1.11). Since u was an arbitrary function in a subspace of dimension ℓ, Theorem 4.1.5 implies that $\mu_{\lambda,\ell} \leq \mu_\ell + Ce^{-r/\lambda}$.

We will now prove the significantly more challenging lower bound. Let $T_0 = (-\frac{3\pi}{4}, -\frac{\pi}{4}) \cup (\frac{\pi}{4}, \frac{3\pi}{4})$ and $T_1 = (-\frac{7\pi}{8}, -\frac{\pi}{8}) \cup (\frac{\pi}{8}, \frac{7\pi}{8})$ be subsets of the torus $\mathbb{T}$, so that $T_0 \subset\subset T_1 \subset\subset \mathbb{T}$. Fix $\chi_0 > 0$, and let $\tilde{\chi} : \mathbb{T} \to [0, \chi_0]$ be a smooth function supported in T_1 such that $\tilde{\chi} = \chi_0$ in $\bar{T}_0$. Let

$$B_\lambda = \tilde{\chi} R_m \tilde{\chi}$$

with R_m an elliptic operator $1 + \lambda^{2m} D_y^{2m}$. This is an operator that is large on T_0 as well as non-negative.

Let $\chi : \mathbb{T} \to [0, 1]$ be a smooth function supported in $(-\frac{3\pi}{4}, \frac{3\pi}{4})$ such that $\chi = 1$ in $[-\frac{\pi}{4}, \frac{\pi}{4}]$. Note that $\text{supp}(\chi') \subset T_0$. Let u be an arbitrary function in $\mathcal{H}^m(\mathbb{T})$. Then,

$$\langle(1-\chi)u, \hat{H}_\lambda^2 \chi u\rangle = \langle(1-\chi)\hat{H}_\lambda u, \chi \hat{H}_\lambda u\rangle + \langle(1-\chi)\hat{H}_\lambda u, [\hat{H}_\lambda, \chi]u\rangle - \langle[\hat{H}_\lambda, \chi]u, \hat{H}_\lambda \chi u\rangle. \tag{4.1.13}$$

The first term on the above right-hand side is non-negative since both χ and $1 - \chi$ are. We now control the remaining terms. Observe that all operators involved are differential operators, and the coefficients of $[\hat{H}_\lambda, \chi]$ vanish wherever χ' does. Thus

$$\langle (1-\chi)\hat{H}_\lambda u, [\hat{H}_\lambda, \chi]u\rangle = \frac{1}{\chi_0^2}\langle (1-\chi)\hat{H}_\lambda \tilde{\chi} u, [\hat{H}_\lambda, \chi]\tilde{\chi} u\rangle.$$

We can similarly insert factors of $\tilde{\chi}/\chi_0$ in the third term of (4.1.13). Since $\hat{H}_\lambda$ is a differential operator of order m and the commutators $[\hat{H}_\lambda, \chi]$ introduce an extra factor of λ, there exists a constant $C_0 > 0$ such that

$$\Re\langle (1-\chi)u, \hat{H}_\lambda^2 \chi u\rangle \geq -\frac{C_0\lambda}{\chi_0^2}(\left\|\lambda^m D_y^m \tilde{\chi} u\right\|^2 + \|\tilde{\chi} u\|^2) \tag{4.1.14}$$

uniformly in $u \in \mathcal{H}^m(\mathbb{T})$. Since $\langle u, B_\lambda u\rangle = \|\tilde{\chi} u\|^2 + \left\|\lambda^m D_y^m \tilde{\chi} u\right\|^2$, we can choose χ_0 sufficiently large so that

$$\langle u, B_\lambda u\rangle + 2\Re\langle (1-\chi)u, \hat{H}_\lambda^2 \chi u\rangle \geq \frac{C}{\chi_0^2}(\left\|\lambda^m D_y^m \tilde{\chi} u\right\|^2 + \|\tilde{\chi} u\|^2) \geq C\, \|u\|_{T_0}^2 \tag{4.1.15}$$

for $C > 0$ as large as necessary. Recall that $\|\cdot\|_{T_0} := \|\cdot\|_{L^2(T_0)\otimes\mathbb{C}^n}$.

By Proposition 4.1.8, we know that the low-energy spectrum of $\hat{H}_\lambda^2$ satisfies

$$\max_{\psi\in\tilde{S}_s;\ \|\psi\|=1} \langle B_\lambda \psi, \psi\rangle = \varepsilon \leq e^{-r/\lambda} \tag{4.1.16}$$

for some $c > 0$, with $\tilde{S}_s = \operatorname{span}(\theta_{\lambda,1}, \dots \theta_{\lambda,s})$. Recall from the definition of s that $\mu_{\lambda,\ell} < E^2$ remains in the (infinite domain) spectral gap for all $\ell \leq s$.

Let us consider the operator $\hat{H}_\lambda^2 + B_\lambda$, also self-adjoint (this is proved as for $\hat{H}_\lambda^2$), with eigenvalues $\nu_{\lambda,j}$. For $1 \leq \ell \leq s$, we have by the min-max principle,

$$\nu_{\lambda,\ell} = \min_{S_\ell} \max_{\psi\in S_\ell,\ \|\psi\|=1} \langle \hat{H}_\lambda^2\psi, \psi\rangle + \langle B_\lambda \psi, \psi\rangle \leq \max_{\psi\in\tilde{S}_\ell,\ \|\psi\|=1} \langle \hat{H}_\lambda^2\psi, \psi\rangle + \langle B_\lambda \psi, \psi\rangle \leq \mu_{\lambda,\ell} + \varepsilon.$$

We may therefore obtain a lower bound for $\nu_{\lambda,\ell}$ now thanks to the regularization B_λ. We have

$$\nu_{\lambda,\ell} \geq \min_{u \in S_{\ell-1}^{\perp},\ \|\psi\|=1} \langle (\hat{H}_\lambda^2 + B_\lambda)u, u\rangle$$

with now $S_{\ell-1}$ the span of $\tilde{\psi}_{\lambda,j}$ for $1 \leq j \leq \ell - 1$ using both families of infinite-domain eigenfunctions properly embedded in the torus.

It follows from Lemma 4.1.9 and (4.1.15) that for $u \in S_{\ell-1}^{\perp}$,

$$\begin{aligned}\langle u, (\hat{H}_\lambda^2 + B_\lambda)u\rangle &= \langle \hat{H}_\lambda^2 \chi u, \chi u\rangle + \langle \hat{H}_\lambda^2 (1-\chi)u, (1-\chi)u\rangle + 2\Re\langle \hat{H}_\lambda^2 \chi u, (1-\chi)u\rangle + \langle B_\lambda u, u\rangle \\ &\geq (\mu_\ell - \eta)\|\chi u\|^2 + (\mu_\ell - \eta)\|(1-\chi)u\|^2 + C\|u\|_{T_0}^2,\end{aligned}$$

with $\eta \leq Ce^{-r/\lambda}$. So, with C large, we have $\langle u, (\hat{H}_\lambda^2 + B_\lambda)u\rangle \geq (\mu_\ell - \eta)\,\|u\|^2$ and thus get

$$\mu_{\lambda,\ell} \geq \nu_{\lambda,\ell} - \varepsilon \geq \mu_\ell - \varepsilon - \eta \geq \mu_\ell - Ce^{-r/\lambda}$$

for all λ sufficiently small.

It remains to prove that $\mu_{\lambda,s+1}$ lies above the support of Υ when λ is small enough. By definition of Υ, there exists $\delta' > 0$ such that $\Upsilon \in \mathcal{C}_c^\infty(-1, E^2 - \delta_0 - \delta')$. Let $u \in \mathcal{H}^m(\mathbb{T})$ such that $u \in S_s^{\perp}$ and $\|u\| = 1$. Take χ as above, with the additional requirement that $\operatorname{supp}(\chi') \subset T_0'$ for some $T_0' \subset T_0$ satisfying $\|u\|_{T_0'}^2 \leq \frac{\delta'}{E^2+1}$. By (4.1.3), which can easily be shown to hold in this one-dimensional setting (see (4.1.5)), it follows that

$$\left\|[\hat{H}_\lambda, \chi](i - \hat{H}_\lambda)^{-1}\right\| \leq C\lambda, \qquad \lambda \in (0, \lambda_0].$$

Writing $[\hat{H}_\lambda, \chi] = [\hat{H}_\lambda, \chi](i - \hat{H}_\lambda)^{-1}(i - \hat{H}_\lambda)$ and $\hat{H}_\lambda \chi = [\hat{H}_\lambda, \chi] + \chi \hat{H}_\lambda$, we use (4.1.13) to conclude that

$$\langle (1-\chi)u, \hat{H}_\lambda^2 \chi u\rangle \geq -C\lambda\Big(\left\|\hat{H}_\lambda u\right\|^2 + \|u\|^2\Big) = -C\lambda\Big(\left\|\hat{H}_\lambda u\right\|^2 + 1\Big).$$

Hence by Lemma 4.1.9, we have

$$\begin{aligned}\langle u, \hat{H}_\lambda^2 u\rangle &= \langle \chi u, \hat{H}_\lambda^2 \chi u\rangle + \langle (1-\chi)u, \hat{H}_\lambda^2 (1-\chi)u\rangle + 2\Re\langle (1-\chi)u, \hat{H}_\lambda^2 \chi u\rangle \\ &\geq (\check{\mu}_{s+1} - Ce^{-r/\lambda}) \|\chi u\|^2 + (\check{\mu}_{s+1} - Ce^{-r/\lambda}) \|(1-\chi)u\|^2 - C\lambda\Big(\Big\|\hat{H}_\lambda u\Big\|^2 + 1\Big),\end{aligned}$$

where $\check{\mu}_{s+1} := \min\{\mu_{s+1}, E^2+1\}$. It follows that $\langle u, \hat{H}_\lambda^2 u\rangle \geq \check{\mu}_{s+1}(\|\chi u\|^2 + \|(1-\chi)u\|^2) - C\lambda$. Since

$$1 = \|u\|^2 = \|\chi u\|^2 + \|(1-\chi)u\|^2 + 2\langle (1-\chi)u, \chi u\rangle \leq \|\chi u\|^2 + \|(1-\chi)u\|^2 + \frac{1}{2}\|u\|_{T_0'}^2,$$

we have shown that

$$\langle u, \hat{H}_\lambda^2 u\rangle \geq \check{\mu}_{s+1} - \frac{1}{2}\check{\mu}_{s+1}\|u\|_{T_0'}^2 - C\lambda \geq \check{\mu}_{s+1} - \frac{1}{2}\delta' - C\lambda.$$

Since u was arbitrary, Theorem 4.1.5 implies that $\mu_{\lambda,s+1} \geq \check{\mu}_{s+1} - \delta'$ for all λ sufficiently small. We know that $\mu_{s+1} \geq E^2 - \delta_0$ by definition, hence $\mu_{\lambda,s+1} \geq E^2 - \delta_0 - \delta'$. This completes the proof. □

Eigenspace approximation. For the following lemma, fix $\lambda \in (0,1]$ and let

$$\{\phi_1, \phi_2, \dots, \phi_s\} \subset \mathcal{H}^m(\mathbb{T})$$

such that $\langle \phi_i, \phi_j\rangle = \delta_{ij}$. For any integers j, k, and ℓ satisfying $1 \leq j \leq k \leq \ell \leq s$, define

$$\alpha_{j,k,\ell} := \Big(1 - \sum_{i=j}^{\ell} |\langle \theta_{\lambda,i}, \phi_k\rangle|^2\Big)^{1/2}, \qquad \alpha_{k,\ell} := \alpha_{1,k,\ell}, \qquad r_j := (\hat{H}_\lambda^2 - \mu_{\lambda,j})\phi_j. \quad (4.1.17)$$

Note that if we denote by $\Pi_{j,\ell}$ the orthogonal projector onto the span of $\{\theta_{\lambda,j}, \dots, \theta_{\lambda,\ell}\}$, then we have

$$\alpha_{j,k,\ell} = \|(I - \Pi_{j,\ell})\phi_k\|. \tag{4.1.18}$$

Lemma 4.1.11. *Let j, k, ℓ be integers satisfying $1 \leq j \leq k \leq \ell \leq s$. Then*

$$\alpha_{j,k,\ell}^2 \leq \|r_k\|^2 (\mu_{\lambda,\ell+1} - \mu_{\lambda,k})^{-2} + \sum_{i=1}^{j-1} \|r_i\|^2 (\mu_{\lambda,j} - \mu_{\lambda,i})^{-2}. \tag{4.1.19}$$

(4.1.18) means ϕ_k lives approximately in $\operatorname{span}(\theta_{\lambda,j}, \theta_{\lambda,j+1}, \dots, \theta_{\lambda,\ell})$ when the right-hand side of (4.1.19) is small.

Proof. For brevity, set $\theta_i := \theta_{\lambda,i}$. We see that $\alpha_{j,k,\ell}^2 = \alpha_{k,\ell}^2 + \sum_{i=1}^{j-1} |\langle \theta_i, \phi_k \rangle|^2$, with

$$\sum_{i=1}^{j-1} |\langle \theta_i, \phi_k \rangle|^2 \leq \sum_{i=1}^{j-1} \Big(1 - \sum_{h=1}^{j-1} |\langle \theta_i, \phi_h \rangle|^2\Big) = \sum_{h=1}^{j-1} \Big(1 - \sum_{i=1}^{j-1} |\langle \theta_i, \phi_h \rangle|^2\Big) = \sum_{h=1}^{j-1} \alpha_{h,j-1}^2.$$

It remains to bound $\alpha_{k,\ell}^2$ and the $\alpha_{h,j-1}^2$. Define $\tilde{\phi}_k := \phi_k - \sum_{i=1}^{\ell} \langle \theta_i, \phi_k \rangle \theta_i$, so that $\langle \theta_i, \tilde{\phi}_k \rangle = 0$ for all $i \in \{1, \dots, \ell\}$, and thus

$$\langle \tilde{\phi}_k, \hat{H}_\lambda^2 \tilde{\phi}_k \rangle \geq \mu_{\lambda,\ell+1} \left\| \tilde{\phi}_j \right\|^2 = \mu_{\lambda,\ell+1} \alpha_{k,\ell}^2 \tag{4.1.20}$$

by Theorem 4.1.5. We also see that $\hat{H}_\lambda^2 \tilde{\phi}_k = \mu_{\lambda,k} \phi_k - \sum_{i=1}^{\ell} \mu_{\lambda,i} \langle \theta_i, \phi_k \rangle \theta_i + r_k$, and hence

$$\begin{aligned} \langle \tilde{\phi}_k, \hat{H}_\lambda^2 \tilde{\phi}_k \rangle &= \mu_{\lambda,k} - \mu_{\lambda,k} \sum_{i=1}^{\ell} |\langle \theta_i, \phi_k \rangle|^2 + \langle \tilde{\phi}_k, r_k \rangle \\ &= \mu_{\lambda,k} \alpha_{k,\ell}^2 + \langle \tilde{\phi}_k, r_k \rangle \leq \mu_{\lambda,k} \alpha_{k,\ell}^2 + \|r_k\| \, \alpha_{k,\ell}. \end{aligned} \tag{4.1.21}$$

Combining (4.1.20) and (4.1.21), we obtain that $\alpha_{k,\ell} \leq \|r_k\| (\mu_{\lambda,\ell+1} - \mu_{\lambda,k})^{-1}$. The same argument proves that $\alpha_{h,j-1} \leq \|r_h\| (\mu_{\lambda,j} - \mu_{\lambda,h})^{-1}$ for all $h \in \{1, 2, \ldots, j-1\}$, and the result is complete. $\square$

We will apply Lemma 4.1.11 to the functions $\phi_j = \tilde{\psi}_{\lambda,j}$. We write $r_j = (\hat{H}^2_\lambda - \mu_j)\tilde{\psi}_{\lambda,j} + (\mu_j - \mu_{\lambda,j})\tilde{\psi}_{\lambda,j}$, meaning that $\|r_j\| \leq \left\|(\hat{H}^2_\lambda - \mu_j)\tilde{\psi}_{\lambda,j}\right\| + |\mu_j - \mu_{\lambda,j}| \leq Ce^{-r/\lambda}$, where the last inequality follows from Proposition 4.1.10 and its proof. Thus if $\min\{\mu_{\lambda,\ell+1} - \mu_{\lambda,k}, \mu_{\lambda,j} - \mu_{\lambda,j-1}\} \geq \delta$ for some $\delta > 0$, then $\alpha^2_{j,k,\ell} \leq C\delta^{-2}e^{-r/\lambda}$. In addition, we have

$$
\begin{aligned}
\beta^2_{j,k,\ell} := \left\|\theta_{\lambda,k} - \sum_{i=j}^{\ell} \langle \tilde{\psi}_{\lambda,i}, \theta_{\lambda,k}\rangle \tilde{\psi}_{\lambda,i}\right\|^2 &= 1 - \sum_{i=j}^{\ell} |\langle \tilde{\psi}_{\lambda,i}, \theta_{\lambda,k}\rangle|^2 \\
&\leq \sum_{i'=j}^{\ell}(1 - \sum_{i=j}^{\ell} |\langle \tilde{\psi}_{\lambda,i}, \theta_{\lambda,i'}\rangle|^2) = \sum_{i=j}^{\ell}(1 - \sum_{i'=j}^{\ell} |\langle \tilde{\psi}_{\lambda,i}, \theta_{\lambda,i'}\rangle|^2) \qquad (4.1.22) \\
&= \sum_{i=j}^{\ell} \alpha^2_{j,i,\ell} \leq C(\ell + 1 - j)\delta^{-2}e^{-r/\lambda}.
\end{aligned}
$$

Lemma 4.1.12. *Let $A_\lambda := \sum_{i=0}^{m-1} a_{\lambda,i}(y)\lambda^i D^i_y$ be an operator on $\mathcal{H}(\mathbb{T})$, for some smooth coefficients $a_{\lambda,i}$ satisfying*

$$
\sum_{i=0}^{m-1} \left\|\lambda^k D^k_y a_{\lambda,i}\right\|_{L^\infty(\mathbb{T})} \leq C'
$$

uniformly in λ for all $k \in \{0, 1, \ldots, m\}$. Let $j \leq \ell$ be positive integers such that $\ell \leq s$ and define $\delta := \min\{\mu_{\lambda,\ell+1} - \mu_{\lambda,\ell}, \mu_{\lambda,j} - \mu_{\lambda,j-1}\}$, where the second argument is ignored if $j = 1$. Then there exist positive constants C and r such that

$$
\Big|\sum_{i=j}^{\ell} \Big(\langle \theta_{\lambda,i}, A_\lambda \theta_{\lambda,i}\rangle - \langle \tilde{\psi}_{\lambda,i}, A_\lambda \tilde{\psi}_{\lambda,i}\rangle\Big)\Big| \leq C\delta^{-1}e^{-r/\lambda}.
$$

Proof. First, we observe that for all $i \in \{1, \dots, s\}$ and $k \in \{0, 1, \dots, m\}$,

$$\left\|\lambda^k D_y^k \nu_{\lambda,i}\right\|^2 \le \left\|\lambda^m D_y^m \nu_{\lambda,i}\right\|^{\frac{2k}{m}} \le C_0\Big(\left\|\hat{H}_\lambda \nu_{\lambda,i}\right\|^2 + C_1\Big)^{\frac{k}{m}} \le C_0(E^2 + C_1)^{\frac{k}{m}}, \qquad \nu = \theta, \tilde{\psi} \tag{4.1.23}$$

uniformly in λ, with the second inequality following from ellipticity of $\hat{H}_\lambda$. We write

$$\sum_{i=j}^{\ell}\Big(\langle\theta_{\lambda,i}, A_\lambda\theta_{\lambda,i}\rangle - \langle\tilde{\psi}_{\lambda,i}, A_\lambda\tilde{\psi}_{\lambda,i}\rangle\Big) =$$
$$\sum_{i=j}^{\ell}\Big(\langle\theta_{\lambda,i} - \sum_{i'=j}^{\ell}\langle\tilde{\psi}_{\lambda,i'}, \theta_{\lambda,i}\rangle\tilde{\psi}_{\lambda,i'}, A_\lambda\theta_{\lambda,i}\rangle - \langle\tilde{\psi}_{\lambda,i}, A_\lambda(\tilde{\psi}_{\lambda,i} - \sum_{i'=j}^{\ell}\langle\theta_{\lambda,i'}, \tilde{\psi}_{\lambda,i}\rangle\theta_{\lambda,i'})\rangle\Big),$$

which implies that

$$\Big|\sum_{i=j}^{\ell}\Big(\langle\theta_{\lambda,i}, A_\lambda\theta_{\lambda,i}\rangle - \langle\tilde{\psi}_{\lambda,i}, A_\lambda\tilde{\psi}_{\lambda,i}\rangle\Big)\Big| \le \sum_{i=j}^{\ell}\Big(\beta_{j,i,\ell}\left\|A_\lambda\theta_{\lambda,i}\right\| + \alpha_{j,i,\ell}\left\|A_\lambda^*\tilde{\psi}_{\lambda,i}\right\|\Big),$$

where $A_\lambda^* := \sum_{i=0}^{m-1}\lambda^i D_y^i a_{\lambda,i}^*(y)$ is the formal adjoint of A_λ. By (4.1.23), we know that the norms of $A_\lambda\nu_{\lambda,i}$ and $A_\lambda^*\nu_{\lambda,i}$ are bounded uniformly in λ, for $\nu = \theta, \tilde{\psi}$. Using (4.1.22) and the corresponding bound for $\alpha_{j,i,\ell}^2$, we conclude that $\Big|\sum_{i=j}^{\ell}\Big(\langle\theta_{\lambda,i}, A_\lambda\theta_{\lambda,i}\rangle - \langle\tilde{\psi}_{\lambda,i}, A_\lambda\tilde{\psi}_{\lambda,i}\rangle\Big)\Big| \le C\delta^{-1}e^{-r/\lambda}$. This completes the result. □

Conductivity approximation. We are now ready to prove Theorem 4.1.1. We will write $\tilde{\sigma}_I$ as a sum of inner products over $\xi \in \lambda\mathbb{Z}$, thus it is helpful to reintroduce the ξ-dependent notation.

Proof of Theorem 4.1.1. Since the coefficients of H_λ are independent of x, we have

$$2\pi\tilde{\sigma}_I = 2\pi\,\mathrm{Tr}\, iQ[H_\lambda, P]\Upsilon(H_\lambda^2) = \sum_{\xi\in\lambda\mathbb{Z}}\sum_{j\in\mathbb{N}}\langle\theta_{\lambda,j,\xi}, i\lambda Q_Y G_\lambda(\xi)\Upsilon(\hat{H}_\lambda^2(\xi))\theta_{\lambda,j,\xi}\rangle,$$

where

$$G_\lambda(\xi) := mM_m\xi^{m-1} + \sum_{j=1}^{m} j\lambda^{m-j}a_{\lambda,j}(y)\xi^{j-1}D_y^{m-j} + \sum_{i+j\le m-1} i\lambda^j a_{\lambda,ij}(y)\xi^{i-1}D_y^j.$$

To obtain G_λ, we used that the contributions from $Q_X[H_\lambda, P]$ of all second and higher order derivatives of P must vanish, as $\int_{\mathbb{T}} Q_X P^{(q)}(x)dx = P^{(q-1)}(\pi/2) - P^{(q-1)}(-\pi/2) = 0$ for all $q > 1$. Using that the $\theta_{\lambda,j,\xi}$ are eigenfunctions of $\hat{H}^2_\lambda(\xi)$, we obtain that

$$2\pi\tilde{\sigma}_I = \sum_{\xi\in\lambda\mathbb{Z}\cap I}\sum_{j=1}^{s_0}\langle\theta_{\lambda,j,\xi}, i\lambda Q_Y G_\lambda(\xi)\theta_{\lambda,j,\xi}\rangle\Upsilon(\mu_{\lambda,j}(\xi)).$$

The next step is to partition the eigenvalues into clusters so that eigenvalues that are nearby belong to the same cluster and the separation between clusters is controlled (bounded from below). We will choose the clusters with diameter sufficiently small so that we can approximate all eigenvalues in a given cluster by the smallest eigenvalue in the cluster, with negligible error. Once Υ is constant over each cluster, we will approximate $\tilde{\sigma}_I$ by a corresponding sum involving the $\tilde{\psi}_{\lambda,j}$ and apply Lemma 4.1.12 to control the error.

By Proposition 4.1.10, the number of eigenvalues of $\hat{H}^2_\lambda(\xi)$ in $\operatorname{supp}(\Upsilon)$ is bounded by $s(\xi)$ uniformly in $\lambda > 0$ sufficiently small and $\xi \in \lambda\mathbb{Z}$. Recall that $s(\xi)$ is the total number of eigenvalues of $\hat{H}^2(\xi)$ and $\hat{H}'^2(\xi)$ lying in $[0, E^2-\delta_0)$, which is itself bounded by s_0 uniformly in ξ and vanishes whenever $\xi \notin I$, with $I \subset \mathbb{R}$ a compact interval; see Proposition 4.1.6. Let $\xi \in \lambda\mathbb{Z}\cap I$ and $\delta := \delta(\lambda)$. Define $k_0(\xi) := 1$, and for all $i \ge 1$ define $k_i(\xi) := \inf\{\ell > k_{i-1}(\xi) : \mu_{\lambda,\ell}(\xi) - \mu_{\lambda,\ell-1}(\xi) \ge \delta \quad \text{or} \quad \ell > s(\xi)\}$. We see that the $k_i(\xi)$ form an increasing sequence of integers, with $k_{J(\xi)}(\xi) = s(\xi)+1$ for some $J(\xi) \in \mathbb{N}$. Define $S_{\xi,j} := \{k_j, \dots, k_{j+1}-1\}$ for all $j \in \{0, 1, \dots, J(\xi)-1\}$, so that $S_{\xi,0}, S_{\xi,1}, \dots, S_{\xi,J(\xi)-1}$ forms a partition of $\{1, 2, \dots, s(\xi)\}$.

Thus we have

$$2\pi\tilde{\sigma}_I = \sum_{\xi\in\lambda\mathbb{Z}\cap I}\sum_{i=0}^{J(\xi)-1}\sum_{j\in S_{\xi,i}} \langle\theta_{\lambda,j,\xi}, i\lambda Q_Y G_\lambda(\xi)\theta_{\lambda,j,\xi}\rangle \Upsilon(\mu_{\lambda,j}(\xi)).$$

By (4.1.23), we see that $|\langle\theta_{\lambda,j,\xi}, G_\lambda(\xi)\theta_{\lambda,j,\xi}\rangle| \le C$ uniformly in λ and ξ. Defining

$$2\pi\tilde{\sigma}_{I,1} := \sum_{\xi\in\lambda\mathbb{Z}\cap I}\sum_{i=0}^{J(\xi)-1}\sum_{j\in S_{\xi,i}} \langle\theta_{\lambda,j,\xi}, i\lambda Q_Y G_\lambda(\xi)\theta_{\lambda,j,\xi}\rangle \Upsilon(\mu_{\lambda,k_i}(\xi)),$$

which replaces each eigenvalue by the smallest eigenvalue in its cluster, we thus obtain that

$$|\tilde{\sigma}_{I,1} - \tilde{\sigma}_I| \le s_0(|I|+1)C \sup_{|x-y|<\delta} |\Upsilon(x) - \Upsilon(y)| \le C\delta \tag{4.1.24}$$

by regularity of Υ, with $|I|$ the length of the interval I. We will now control the error from replacing the periodic eigenfunctions $\theta_{\lambda,j,\xi}$ in $\tilde{\sigma}_{I,1}$ by the truncations $\tilde{\psi}_{\lambda,j,\xi}$. Namely, it follows from Lemma 4.1.12 that

$$2\pi\tilde{\sigma}_{I,2} := \sum_{\xi\in\lambda\mathbb{Z}\cap I}\sum_{i=0}^{J(\xi)-1}\sum_{j\in S_{\xi,i}} \langle\tilde{\psi}_{\lambda,j,\xi}, i\lambda Q_Y G_\lambda(\xi)\tilde{\psi}_{\lambda,j,\xi}\rangle \Upsilon(\mu_{\lambda,k_i}(\xi))$$

satisfies $|\tilde{\sigma}_{I,2} - \tilde{\sigma}_{I,1}| \le C\delta^{-1}e^{-r/\lambda}$. Here, we have used the extra factor of λ that appears in the inner product to cancel the λ^{-1} scaling of the number of terms in the sum over ξ. We can simplify $\tilde{\sigma}_{I,2}$ as

$$2\pi\tilde{\sigma}_{I,2} = \sum_{\xi\in\lambda\mathbb{Z}\cap I}\sum_{i=0}^{J(\xi)-1}\sum_{j\in S'_{\xi,i}} \langle\tilde{\psi}_{\lambda,j,\xi}, i\lambda G_\lambda(\xi)\tilde{\psi}_{\lambda,j,\xi}\rangle \Upsilon(\mu_{\lambda,k_i}(\xi)),$$

with $S'_{\xi,i}$ containing only the indices j in $S_{\xi,i}$ such that $\operatorname{supp}(\tilde{\psi}_{j,\xi,\lambda}) \cap \operatorname{supp} Q_Y \neq \emptyset$. That is, $S'_{\xi,i} \subseteq S_{\xi,i}$ and $\bigcup_{i=0}^{J(\xi)-1} S'_{\xi,i} = R_\xi$. Here, we used the fact that $Q_Y = 1$ on $\operatorname{supp}(\tilde{\psi}_{\lambda,j,\xi})$

for all $j \in S'_{\xi,i}$.

Note that for all $\xi \in \lambda\mathbb{Z} \cap I$, $i \in \{1, \ldots, J(\xi) - 1\}$ and $j \in S'_{\xi,i}$, we have

$$|\mu_j(\xi) - \mu_{\lambda,k_i}(\xi)| \leq |\mu_j(\xi) - \mu_{\lambda,j}(\xi)| + |\mu_{\lambda,j}(\xi) - \mu_{\lambda,k_i}(\xi)| \leq C(e^{-r/\lambda} + \delta)$$

by Proposition 4.1.10. Thus, by the same logic used to justify (4.1.24), we know that

$$2\pi\tilde{\sigma}_{I,3} := \sum_{\xi \in \lambda\mathbb{Z} \cap I} \sum_{i=0}^{J(\xi)-1} \sum_{j \in S'_{\xi,i}} \langle \tilde{\psi}_{\lambda,j,\xi}, i\lambda G_\lambda(\xi)\tilde{\psi}_{\lambda,j,\xi} \rangle \Upsilon(\mu_j(\xi))$$

satisfies $|\tilde{\sigma}_{I,3} - \tilde{\sigma}_{I,2}| \leq C(e^{-r/\lambda} + \delta)$.

We now express $\tilde{\sigma}_{I,3}$ in terms of functions in $\mathcal{H}(\mathbb{R})$ as

$$2\pi\tilde{\sigma}_{I,3} = \lambda \sum_{\xi \in \lambda\mathbb{Z} \cap I} \sum_{i=0}^{J(\xi)-1} \sum_{j \in S'_{\xi,i}} (\Lambda_{\lambda,0}\psi_{\lambda,j,\xi}, \hat{G}(\xi)\Lambda_{\lambda,0}\psi_{\lambda,j,\xi})\Upsilon(\mu_j(\xi)),$$

where $\hat{G}(\xi) = \mathrm{Op}(\tau_\xi)$ with $\tau_\xi(y,\zeta) := \partial_\xi \sigma(y,\xi,\zeta)$ Hermitian-valued. Defining

$$2\pi\tilde{\sigma}_{I,4} := \lambda \sum_{\xi \in \lambda\mathbb{Z} \cap I} \sum_{i=0}^{J(\xi)-1} \sum_{j \in S'_{\xi,i}} (\psi_{j,\xi}, \hat{G}(\xi)\psi_{j,\xi})\Upsilon(\mu_j(\xi)),$$

it follows that

$$\begin{aligned} 2\pi(\tilde{\sigma}_{I,4} - \tilde{\sigma}_{I,3}) = \lambda \sum_{\xi \in \lambda\mathbb{Z} \cap I} \sum_{i=0}^{J(\xi)-1} \sum_{j \in S'_{\xi,i}} \Big(&(\psi_{j,\xi} - \Lambda_{\lambda,0}\psi_{\lambda,j,\xi}, \hat{G}(\xi)\psi_{j,\xi}) \\ &+ (\Lambda_{\lambda,0}\psi_{\lambda,j,\xi}, \hat{G}(\xi)(\psi_{j,\xi} - \Lambda_{\lambda,0}\psi_{\lambda,j,\xi}))\Big)\Upsilon(\mu_j(\xi)), \end{aligned}$$

so that

$$2\pi|\tilde{\sigma}_{I,4}-\tilde{\sigma}_{I,3}| \leq \lambda \sum_{\xi\in\lambda\mathbb{Z}\cap I} \sum_{i=0}^{J(\xi)-1} \sum_{j\in S'_{\xi,i}} \Big(|||\psi_{j,\xi}-\Lambda_{\lambda,0}\psi_{\lambda,j,\xi}||| \, \Big|\Big|\Big|\hat{G}(\xi)\psi_{j,\xi}\Big|\Big|\Big| + \Big|\Big|\Big|\hat{G}(\xi)\Lambda_{\lambda,0}\psi_{\lambda,j,\xi}\Big|\Big|\Big| \, |||\psi_{j,\xi}-\Lambda_{\lambda,0}\psi_{\lambda,j,\xi}||| \Big) \|\Upsilon\|_\infty .$$

Note that $\hat{G}(\xi)\in \mathrm{Op}(S^m_{1,0})$ and $(i-\hat{H}(\xi))^{-1}\in \mathrm{Op}(S^{-m}_{1,0})$ by (H1), hence $\hat{G}(\xi)(i-\hat{H}(\xi))^{-1}$ is bounded for all $\xi\in I$. The norm is continuous as a function of ξ in I a compact interval, meaning that $\left\|\hat{G}(\xi)(i-\hat{H}(\xi))^{-1}\right\|$ is bounded uniformly in $\xi\in I$. Writing

$$\hat{G}(\xi)\psi_{j,\xi} = \hat{G}(\xi)(1+\hat{H}^2(\xi))^{-1}(1+\hat{H}^2(\xi))\psi_{j,\xi}$$

with $\Big|\Big|\Big|(1+\hat{H}^2(\xi))\psi_{j,\xi}\Big|\Big|\Big| \leq 1+E^2$ for all $j\leq s(\xi)$, it follows from (4.1.11) that $|\tilde{\sigma}_{I,4}-\tilde{\sigma}_{I,3}|\leq Ce^{-r/\lambda}$.

So far, we have shown that $|\tilde{\sigma}_{I,4}-\tilde{\sigma}_I|\leq C(\delta^{-1}e^{-r/\lambda}+e^{-r/\lambda}+\delta)$, for some positive constants C and r. Therefore, setting $\delta := e^{-r/2\lambda}$, we obtain that $|\tilde{\sigma}_{I,4}-\tilde{\sigma}_I|\leq Ce^{-r/2\lambda}$.

Finally, we recall from [7, 10] that

$$2\pi\sigma_I = \int_{\mathbb{R}} \sum_{i=0}^{J(\xi)-1} \sum_{j\in S'_{\xi,i}} (\psi_{j,\xi}, \hat{G}(\xi)\psi_{j,\xi})\Upsilon(\mu_j(\xi))d\xi,$$

with the above integrand a smooth, compactly supported function of ξ by Proposition 4.1.6. It is well known (see, e.g. [60]) that such integrals can be approximated by sampling over a uniform grid of size λ, with convergence faster than any power of λ. We conclude that $|\tilde{\sigma}_{I,4}-\sigma_I|\leq C\lambda^p$, and the proof is complete. □

Observe that $|\tilde{\sigma}_{I,4}-\sigma_I|$ is the only error term that does not converge exponentially in λ. Thus if it were not for the approximation of the integral over ξ by a discrete sum, we would get exponential convergence of the periodic conductivity to its corresponding infinite-space value.

4.2 Stability of physical observable

The aim of this section is to prove stability of $\tilde{\sigma}_I(H_\lambda)$ under perturbations in the limit $\lambda \to 0$, with H_λ given by (4.1.1) and $\tilde{\sigma}_I$ by (4.0.3). We consider perturbations of the form $V_\lambda := \sum_{i+j\le m-1} \lambda^{i+j} v_{\lambda,ij}(x,y) D_x^i D_y^j$, where the $v_{\lambda,ij}$ are smooth matrix-valued functions that make V_λ a symmetric differential operator on $L^2(\mathbb{T}^2)\otimes\mathbb{C}^n$. Assume that $\sum_{i,j} \left\|v_{\lambda,ij}\right\|_{L^\infty} \le C$ uniformly in λ. Suppose there exists a closed set $S_1 \subset \mathbb{T}^2$ such that $\cup_{i,j}\operatorname{supp}(v_{\lambda,ij}) \subset S_1$ for all $\lambda \in (0, \lambda_0]$ and $\operatorname{supp}((1-Q)P') \cap S_1 = \emptyset$.

The condition on the sup-norm of $v_{\lambda,ij}$ guarantees that the coefficients of $H_\lambda + V_\lambda$ are bounded uniformly in λ. As in section 4.1 and combined with the assumption that V_λ is symmetric, this ensures that $H_\lambda + \mu V_\lambda$ is uniformly elliptic (in the sense of Proposition 4.1.2) and hence self-adjoint. Note that $L^\infty-$bounds on derivatives of the $v_{\lambda,ij}$ are not necessary since V_λ has no leading order terms. The condition on the support of $v_{\lambda,ij}$ is natural as it ensures that the perturbation is close to the domain wall of interest and well separated from the spurious domain wall introduced by the periodization. It allows us to express $\tilde{\sigma}_I(H_\lambda + V_\lambda) - \tilde{\sigma}_I(H_\lambda)$ as the integral over a product of operators, two of which are differential operators with disjoint support (see the proof of Theorem 4.2.1 below). Note that the assumption $\operatorname{supp}((1-Q)P') \cap S_1 = \emptyset$ could easily be replaced by $\operatorname{supp}(QP') \cap S_1 = \emptyset$.

Our main stability result is the following

Theorem 4.2.1. *Take H_λ and V_λ as above. Then for all $N \in \mathbb{N}$,*

$$|\tilde{\sigma}_I(H_\lambda + V_\lambda) - \tilde{\sigma}_I(H_\lambda)| \le C_N \lambda^N.$$

This result, combined with that of Theorem 4.1.1, shows that the periodic approximation of the conductivity enjoys a spectral (almost exponential) convergence property with $\sigma_I(H)-$

$\tilde{\sigma}_I(H_\lambda + V_\lambda)$ being of order λ^p for any $p \geq 0$.

The rest of this section is devoted to proving Theorem 4.2.1. For $\varepsilon \in \{0,1\}$, define $H_{\lambda,\varepsilon} := H_\lambda + \varepsilon V_\lambda$.[2] The arguments from section 4.1 can easily be adapted to prove that the $H_{\lambda,\varepsilon}$ are self-adjoint for all λ, with

$$\left\|H_{\lambda,\varepsilon} f\right\|^2 \geq C_1 \left\|f\right\|_{\lambda,m}^2 - C_2 \left\|f\right\|^2, \qquad \left\|\lambda^{|\alpha|} D^\alpha (i - H_{\lambda,\varepsilon})^{-1}\right\| \leq C \tag{4.2.1}$$

for all $f \in \mathcal{H}^m(\mathbb{T}^2)$ and $|\alpha| \leq m$ uniformly in $\lambda \in (0, \lambda_0]$.

We first show that $\tilde{\sigma}_I$ is unchanged for Q replaced by $Q-1$, using $1 = Q + 1 - Q$ and the following result:

Lemma 4.2.2. *Let H be a self-adjoint linear operator and $\Phi \in \mathcal{C}_c^\infty(\mathbb{R})$ such that $[H,P]\Phi(H)$, $H\Phi(H)$, and $\Phi(H)$ are trace-class. Then $\operatorname{Tr} i[H,P]\Phi(H) = 0$.*

Proof. Since P is bounded, $PH\Phi(H)$ is trace class, and thus so is $HP\Phi(H) = [H,P]\Phi(H) + PH\Phi(H)$. Using Lemma 2.1.2 (which still applies in the periodic setting) and cyclicity of the trace, we have

$$\begin{aligned}\operatorname{Tr} i[H,P]\Phi(H) = \operatorname{Tr} i[\Psi(H),P]\Phi(H) &= \operatorname{Tr} i\Psi(H)P\Phi(H) - \operatorname{Tr} iP\Psi(H)\Phi(H) \\ &= \operatorname{Tr} iP\Phi(H)\Psi(H) - \operatorname{Tr} iP\Psi(H)\Phi(H) = 0,\end{aligned}$$

as desired. □

Clearly, and thankfully, the assumptions of Lemma 4.2.2 were not satisfied in the infinite-space setting. However, due to compactness of the torus, these assumptions hold in the periodic setting for the Hamiltonians we consider as we show below. The filter Q that appears in $\tilde{\sigma}_I$ thus allows for non-vanishing conductivities.

We now bound the trace-norm of appropriate functionals of the $H_{\lambda,\varepsilon}$.

2. Not to be confused with the operators $H_{\lambda,\mu}$ from section 4.1.

Proposition 4.2.3. *For all $\Phi \in \mathcal{C}_c^\infty(\mathbb{R})$ and $\varepsilon \in \{0,1\}$, there is a positive constant C such that $\left\|\Phi(H_{\lambda,\varepsilon})\right\|_1 \leq C\lambda^{-2}$ uniformly in $\lambda \in (0,\lambda_0]$.*

Proof. Let $M > 0$ such that $\Phi \in \mathcal{C}_c^\infty(-M,M)$. For $(\xi,\zeta) \in \mathbb{Z}^2$ and $j \in \{1,2,\dots,n\}$, define $\phi_{\xi,\zeta,j}(x,y) = \frac{1}{2\pi}e^{i(\xi x+\zeta y)}v_j$, where v_j is the jth column of the $n \times n$ identity matrix. Thus the $\phi_{\xi,\zeta,j}$ form an orthonormal basis for $\mathcal{H}(\mathbb{T}^2)$. Let $k \in \mathbb{N}$ and define $S_k := (\mathbb{Z} \cap [-k+1, k-1])^2 \times (\mathbb{N} \cap [1,n])$ and $T_k := (\mathbb{Z}^2 \times (\mathbb{N} \cap [1,n])) \setminus S_k$. Let $u = \sum_{(\xi,\zeta,j)\in T_k} c_{\xi,\zeta,j}\phi_{\xi,\zeta,j}$, with $(c_{\xi,\zeta,j}) \subset \mathbb{C}$ chosen so that $u \in \mathcal{H}^m(\mathbb{T}^2)$. It follows that

$$\begin{aligned}
\|u\|_{\lambda,m}^2 &= \sum_{|\alpha|\leq m} \sum_{(\xi,\zeta,j)\in T_k} |c_{\xi,\zeta,j}|^2 (\lambda\xi)^{2\alpha_1}(\lambda\zeta)^{2\alpha_2} \\
&\geq (\lambda k)^{2m} \sum_{(\xi,\zeta,j)\in T_k} |c_{\xi,\zeta,j}|^2 = (\lambda k)^{2m} \|u\|^2 .
\end{aligned}$$

To justify the inequality, we sum over $\alpha \in \{(m,0),(0,m)\}$ and use the fact that for all $(\xi,\zeta,j) \in T_k$, $\xi \geq k$ or $\zeta \geq k$. Thus if $(\lambda k)^{2m} \geq C_1^{-1}(M^2 + C_2)$, then (4.2.1) implies that $\left\|H_{\lambda,\varepsilon}u\right\|^2 \geq M^2 \|u\|^2$. Since u is an arbitrary function in $\operatorname{span}(\phi_{\xi,\zeta,j} : (\xi,\zeta,j) \in S_k)^\perp$, Theorem 4.1.5 implies that the spectrum of $H_{\lambda,\varepsilon}^2$ in $(-\infty, M^2)$ consists entirely of eigenvalues, and the number of these eigenvalues is bounded by $C\lambda^{-2}$ for some $C > 0$. Hence the number of eigenvalues of $H_{\lambda,\varepsilon}$ in $(-M,M)$ is also bounded by $C\lambda^{-2}$, and the result follows. $\square$

We are now ready to prove the main result of this section. Below we bound the difference of conductivities $|\tilde{\sigma}_I(H_{\lambda,1}) - \tilde{\sigma}_I(H_{\lambda,0})|$ by the product of a trace-norm and operator-norm. Proposition 4.2.3 provides a ($\lambda-$dependent) bound on the involved trace-norm. Combined with (4.2.1), this bound verifies the assumptions of Lemma 4.2.2. We conclude by showing that the operator norm goes to zero faster than any power of λ.

Proof of Theorem 4.2.1. Let $W = W(x,y)$ be a smooth point-wise multiplication operator proportional to the identity matrix. By (4.2.1), we have

$$\begin{aligned}\left\|[H_{\lambda,\varepsilon'},W](z-H_{\lambda,\varepsilon})^{-1}\right\| &= \left\|[V_\lambda,W](i-H_{\lambda,\varepsilon})^{-1}(i-H_{\lambda,\varepsilon})(z-H_{\lambda,\varepsilon})^{-1}\right\| \\ &\leq \left\|[V_\lambda,W](i-H_{\lambda,\varepsilon})^{-1}\right\|\left(1+|i-z|\left\|(z-H_{\lambda,\varepsilon})^{-1}\right\|\right) \\ &\leq C|\Im z|^{-1}\lambda \end{aligned}\tag{4.2.2}$$

for all $(\varepsilon,\varepsilon')\in\{0,1\}^2$ uniformly in $\lambda\in(0,\lambda_0]$ and $z\in Z\setminus\{\Im z=0\}$, where $Z:=[E_1,E_2]\times[-2,2]\subset\mathbb{C}$. Similarly,

$$\left\|V_\lambda(z-H_{\lambda,\varepsilon})^{-1}\right\|\leq C|\Im z|^{-1}\tag{4.2.3}$$

uniformly in $\lambda\in(0,\lambda_0]$ and $z\in Z\setminus\{\Im z=0\}$. Let $\Phi\in\mathcal{C}_c^\infty(E_1,E_2)$ such that $\Phi\varphi'=\varphi'$. Applying Proposition 4.2.3 to the compactly supported function $x\mapsto(i-x)\Phi(x)$, we obtain by (4.2.2) that

$$\left\|[H_{\lambda,\varepsilon},W]\Phi(H_{\lambda,\varepsilon})\right\|_1\leq\left\|[H_{\lambda,\varepsilon},W](i-H_{\lambda,\varepsilon})^{-1}\right\|\left\|(i-H_{\lambda,\varepsilon})\Phi(H_{\lambda,\varepsilon})\right\|_1\leq C\lambda^{-1}\tag{4.2.4}$$

uniformly in λ.

Fix $N\in\mathbb{N}$ and define $\tilde{Q}:=Q-1$. With Proposition 4.2.3 and (4.2.4), we have verified that $H_{\lambda,\varepsilon}$ satisfies the assumptions of Lemma 4.2.2 for $\varepsilon\in\{0,1\}$, hence $\tilde{\sigma}_I(H_{\lambda,\varepsilon})=\operatorname{Tr} i\tilde{Q}[H_{\lambda,\varepsilon},P]\varphi'(H_{\lambda,\varepsilon})$. By assumption, $\tilde{Q}[V_\lambda,P]=0$, so that

$$\tilde{\sigma}_I(H_{\lambda,\varepsilon})=\operatorname{Tr} i\tilde{Q}[H_{\lambda,0},P]\varphi'(H_{\lambda,\varepsilon}).$$

Moreover, there exists a (λ-independent) smooth point-wise multiplication operator R proportional to the identity matrix, such that $R=1$ on $\operatorname{supp}(\tilde{Q}P')$ and $\operatorname{supp}(R)\cap S_1=\emptyset$. It follows that

$$\begin{aligned}\tilde{\sigma}_I(H_{\lambda,0}) - \tilde{\sigma}_I(H_{\lambda,1}) &= \operatorname{Tr} iR\tilde{Q}[H_{\lambda,0}, P](\varphi'(H_{\lambda,0}) - \varphi'(H_{\lambda,1})) \\ &= \operatorname{Tr} i\tilde{Q}[H_{\lambda,0}, P]\Phi(H_{\lambda,0})(\varphi'(H_{\lambda,0}) - \varphi'(H_{\lambda,1}))R \\ &\quad + \operatorname{Tr} i\tilde{Q}[H_{\lambda,0}, P]R(\Phi(H_{\lambda,0}) - \Phi(H_{\lambda,1}))\varphi'(H_{\lambda,1}) =: \Delta_0 + \Delta_1,\end{aligned}$$

where we have used cyclicity of the trace to move R to the right-most position on the second line. By the Helffer-Sjöstrand formula, we see that

$$(\varphi'(H_{\lambda,0}) - \varphi'(H_{\lambda,1}))R = \frac{1}{\pi}\int_Z \bar{\partial}\tilde{\varphi'}(z)(z - H_{\lambda,1})^{-1}V_\lambda(z - H_{\lambda,0})^{-1}Rd^2z.$$

Since $\operatorname{supp}(R)$ and S_1 are closed and disjoint sets, there exists a (λ-independent) collection $\{W_0, W_1, \ldots, W_N\}$ of smooth, point-wise multiplication operators proportional to the identity matrix such that $W_jV_\lambda = 0$ and $W_{j+1}W_j = W_j$ for all j and λ, with $W_0 := R$. Using the fact that $[(z - H_{\lambda,0})^{-1}, W_j] = (z - H_{\lambda,0})^{-1}[H_{\lambda,0}, W_j](z - H_{\lambda,0})^{-1}$, we obtain that

$$\begin{aligned}V_\lambda(z - H_{\lambda,0})^{-1}R &= V_\lambda[(z - H_{\lambda,0})^{-1}, W_0] = V_\lambda(z - H_{\lambda,0})^{-1}[H_{\lambda,0}, W_0](z - H_{\lambda,0})^{-1} \\ &= V_\lambda(z - H_{\lambda,0})^{-1}W_1[H_{\lambda,0}, W_0](z - H_{\lambda,0})^{-1} \\ &= V_\lambda(z - H_{\lambda,0})^{-1}[H_{\lambda,0}, W_1](z - H_{\lambda,0})^{-1}[H_{\lambda,0}, W_0](z - H_{\lambda,0})^{-1} \\ &= V_\lambda(z - H_{\lambda,0})^{-1}W_2[H_{\lambda,0}, W_1](z - H_{\lambda,0})^{-1}[H_{\lambda,0}, W_0](z - H_{\lambda,0})^{-1} \\ &= \quad \ldots \\ &= V_\lambda(z - H_{\lambda,0})^{-1}[H_{\lambda,0}, W_N](z - H_{\lambda,0})^{-1}[H_{\lambda,0}, W_{N-1}](z - H_{\lambda,0})^{-1} \\ &\qquad\qquad \ldots (z - H_{\lambda,0})^{-1}[H_{\lambda,0}, W_0](z - H_{\lambda,0})^{-1}.\end{aligned}$$

By (4.2.2), $\|[H_{\lambda,0}, W_j](z - H_{\lambda,0})^{-1}\| \le C_j|\Im z|^{-1}\lambda$ for every j. Thus by (4.2.3) and the rapid decay of $\bar{\partial}\tilde{\varphi'}$ near the real axis, it follows that $\|(\varphi'(H_{\lambda,0}) - \varphi'(H_{\lambda,1}))R\| \le C\lambda^{N+1}$.

Using (4.2.4), we conclude that

$$|\Delta_0| \leq \left\|\tilde{Q}[H_{\lambda,0}, P]\Phi(H_{\lambda,0})\right\|_1 \left\|(\varphi'(H_{\lambda,0}) - \varphi'(H_{\lambda,1}))R\right\| \leq C\lambda^N.$$

By cyclicity of the trace, $\Delta_1 = \operatorname{Tr} i\varphi'(H_{\lambda,1})\tilde{Q}[H_{\lambda,0}, P]R(\Phi(H_{\lambda,0}) - \Phi(H_{\lambda,1}))$, so that the above argument can be repeated to obtain the same bound for $|\Delta_1|$. We conclude that $|\tilde{\sigma}_I(H_{\lambda,0}) - \tilde{\sigma}_I(H_{\lambda,1})| \leq C\lambda^N$, and the proof is complete. $\square$

4.3 Applications

We apply the main results from Sections 4.1 and 4.2 to the Hamiltonians from Section 2.3 that are differential operators. We have already verified that these systems satisfy (H1), thus the only thing left to check is the anti-commutation relations of the leading order terms (4.0.2).

2×2 **Dirac system** (2.3.1). We have $H = D_x\sigma_1 + D_y\sigma_2 + m(y)\sigma_3$, meaning that we can take $M_0 = \sigma_2$, $M_1 = \sigma_1$, and $a_{00}(y) = m(y)\sigma_3$. Since the σ_j are nonsingular and $\{\sigma_1, \sigma_2\} = 0$, (4.0.2) holds. It follows that $|\tilde{\sigma}_I(H_\lambda) - \sigma_I(H)| \leq C_p\lambda^p$ as $\lambda \to 0$, for any p. Moreover, $|\tilde{\sigma}_I(H_\lambda) - \tilde{\sigma}_I(H_\lambda + V_\lambda)| \leq C_p\lambda^p$ for all smooth Hermitian-valued point-wise multiplication operators $V_\lambda = V_\lambda(x, y)$ such that $\|V_\lambda\|_{L^\infty} \leq C$ uniformly in λ, and that satisfy $S_1 \cap \operatorname{supp}(1 - Q) = \emptyset$ for some closed set S_1 containing $\cup_\lambda \operatorname{supp}(V_\lambda)$.

p**-wave superconductor model** (2.3.2). We can take $M_0 = M_2 = \frac{1}{2m}\sigma_1$, which takes care of all leading order terms. Since σ_1 is non-singular, (4.0.2) holds. It follows that $|\tilde{\sigma}_I(H_\lambda) - \sigma_I(H)| \leq C_p\lambda^p$ for any p. We also have $|\tilde{\sigma}_I(H_\lambda) - \tilde{\sigma}_I(H_\lambda + V_\lambda)| \leq C_p\lambda^p$ for all Hermitian-valued first-order differential operators $V_\lambda := \sum_{i+j\leq 1} \lambda^{i+j} v_{\lambda,ij}(x, y) D_x^i D_y^j$ with smooth coefficients $v_{\lambda,ij}$ such that $\sum_{i,j} \left\|v_{\lambda,ij}\right\|_{L^\infty} \leq C$ and $\cup_{i,j} \operatorname{supp}(v_{\lambda,ij}) \subset S_1$ uniformly in λ, for some closed set S_1 satisfying $S_1 \cap \operatorname{supp}(1 - Q) = \emptyset$.

d**-wave superconductor model** (2.3.3). Take $M_0 = M_2 = \frac{1}{2m}\sigma_1$, $a_0 = c_0\sigma_2$, $a_1(y) =$

$c(y)\sigma_3$, $a_2 = -c_0\sigma_2$. Since σ_1 is nonsingular and $\{\sigma_1, \sigma_j\} = 0$ for $j \in \{2, 3\}$, (4.0.2) holds. The following conclusions are the same as those for the p-wave superconductor model above.

4.4 Numerical simulations

To illustrate the stability (or not) of interface conductivities, we present numerical simulations of the 2×2 Dirac and p-wave superconductor models from section 2.3, as well as models of equatorial waves analyzed in section 2.3 (see also [10]). We discretize a grid of size $L_x \times L_y = 24 \times 24$ uniformly into $N_x \times N_y = 64 \times 64$ grid points and impose periodic boundary conditions. Point-wise multiplication operators are represented as diagonal matrices, and derivatives $\tilde{D}_\alpha \approx \frac{1}{i}\partial_\alpha$ $(\alpha = x, y)$ are computed in the Fourier basis $\tilde{D}_\alpha = F_\alpha^{-1}\Lambda_\alpha F_\alpha$, where F_α is the discrete Fourier transform with respect to direction α, and

$$\Lambda_\alpha = \frac{2\pi}{N_\alpha L_\alpha} \operatorname{diag}\Big(-\frac{N_\alpha}{2}, -\frac{N_\alpha}{2} + 1, \dots, \frac{N_\alpha}{2} - 1\Big).$$

Note that F_α is unitary, so that $F_\alpha^{-1} = F_\alpha^*$. We refer the reader to [84] for more details on spectral methods and their accuracy.

As in section 4.1, we define the conductivity by

$$\tilde{\sigma}_I(H) := \operatorname{Tr} iQ[H, P]\varphi'(H),$$

where $P = P(x)$ and $Q = Q(x, y) = Q_X(x)Q_Y(y)$ are point-wise multiplication operators satisfying

$$P(x) = \begin{cases} 1, & \delta_x \le x \le 3L_x/8 \\ 0, & -3L_x/8 \le x \le -\delta_x \end{cases} \qquad \text{and} \qquad Q_\Theta(\theta) = \begin{cases} 1, & |\theta| \le L_\theta/4 \\ 0, & |\theta| \ge L_\theta/4 + \delta_\theta \end{cases},$$

for some $0 < \delta_\theta \ll L_\theta/4$. The Hamiltonians are periodized so that the y dependent terms

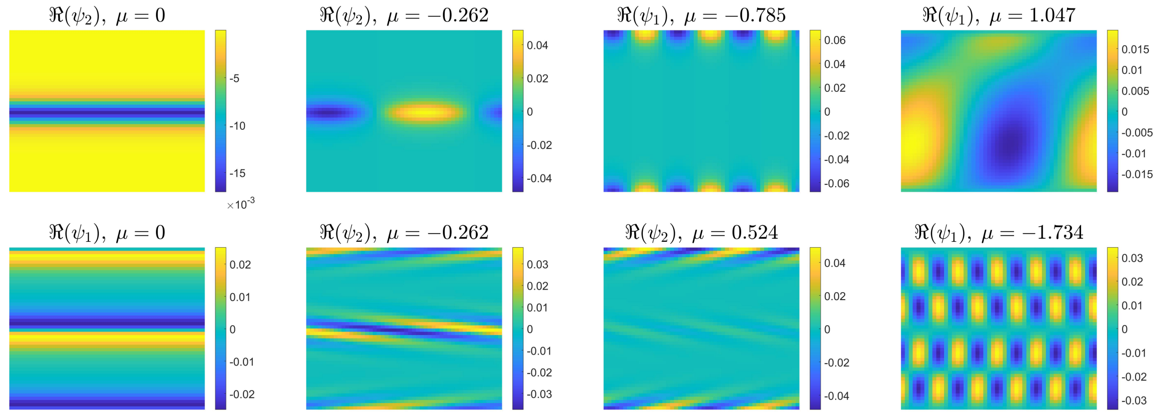

Figure 4.1: Eigenfunctions of the periodic 2×2 Dirac Hamiltonian (top) and p-wave superconductor (bottom) models. First three columns: edge states localized at the $y = 0$ and $y = \pm L_y/2$ interfaces; far right: bulk states that do not contribute to the conductivity. The plotted vector components and corresponding eigenvalues are labeled.

($m(y)$ for the 2×2 Dirac system and $c(y)$ for the p-wave superconductor) are equal to 1 whenever $\delta' \le y \le L_y/2 - \delta'$ and -1 for $-L_y/2 + \delta' \le y \le -\delta'$, and are smoothly connected in between. Here, δ' is a positive constant that is small relative to L_y, but large enough for the interval $(-\delta', \delta')$ to contain at least 3 grid points. The eigenvalues of H in the support of φ' (and the corresponding eigenvectors) are computed using the "eigs" command in MATLAB. Since the number of these eigenvalues is typically much smaller than the dimension of H, we avoid the computational expense of a full spectral decomposition.

For the 2×2 models, we consider perturbations of the form

$$V(x,y) = (\hat{n} \cdot \vec{\sigma}) v(x,y), \qquad v(x,y) = \begin{cases} r \exp(-a^2/(a^2 - x^2 - y^2)), & x^2 + y^2 < a^2, \\ 0, & \text{else}, \end{cases}$$

where $\hat{n} \in \mathbb{R}^4$ is a unit normal vector and $\vec{\sigma} = (\sigma_0, \sigma_1, \sigma_2, \sigma_3)$. Here, the σ_j are the Pauli matrices (with σ_0 the 2×2 identity matrix). We observe that $\tilde{\sigma}_I$ is stable with respect to such perturbations. Namely, if we fix the support of v to lie well within $\mathrm{supp}(Q)$ while increasing the amplitude of that perturbation, the conductivity does not change by much (even if the

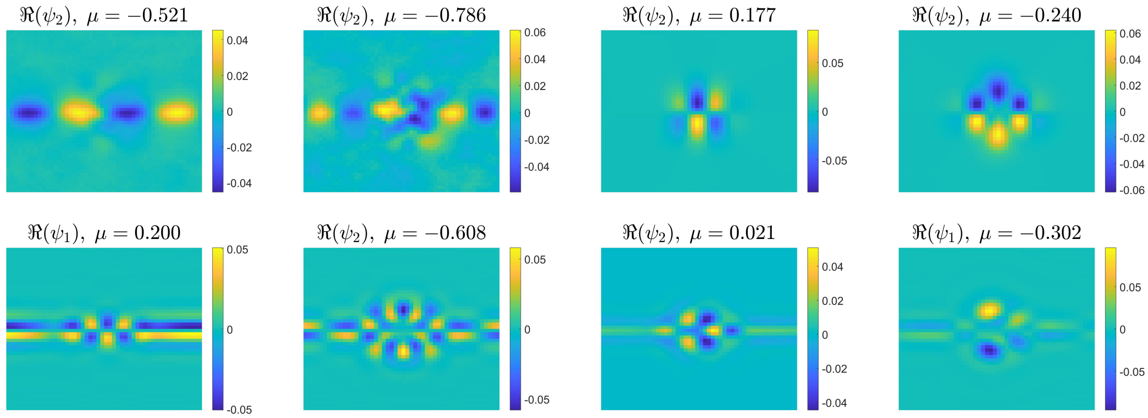

Figure 4.2: Perturbed eigenfunctions of the 2×2 Dirac (top) and p-wave superconductor (bottom) models. For all plots, $r = 2$ and $a = 7.5$. We see a mix of propagating and evanescent modes. Despite the qualitative differences between the perturbed and unperturbed eigenfunctions, the conductivity remains approximately the same.

amplitude is very large). Similarly, for a fixed amplitude, the conductivity remains close to its original value until v becomes highly delocalized. See Figure 4.3 (left), where we have plotted the dependence of the conductivity on the perturbation strength and localization for the 2×2 Dirac and p-wave superconductor models. Note that for many other choices of parameters, the conductivity remains within 2% of its unperturbed value for values of r and a much larger than 10. The empirical stability of $\tilde{\sigma}_I$ is entirely consistent with the theoretical results from earlier sections.

We present examples of computed eigenfunctions for the 2×2 Dirac and p-wave superconductor models in Figures 4.1 and 4.2. We observe that perturbations V of the above form strongly alter the edge states. They are no longer a superposition of terms of the form $e^{i\xi x}\psi(y)$ and we even recognise localized modes (see top right of Figure 4.2) that do not contribute to the conductivity. Thus the robustness of $\tilde{\sigma}_I$ observed in Figure 4.3 occurs in spite of the instability of the eigenfunctions with respect to perturbations.

One may also consider filters $Q_{\Delta_X,\Delta_Y}(x,y) = Q_{\Delta_X}(x)Q_{\Delta_Y}(y)$ with different centers,

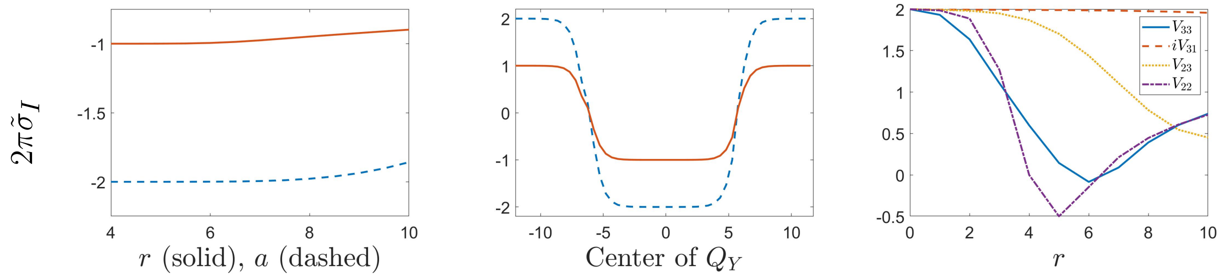

Figure 4.3: The left panel demonstrates the numerical stability of $\tilde{\sigma}_I$ for the 2×2 Dirac (solid line) and p-wave superconductor (dashed line) models. For the solid line, we fixed $a = 7.5$ (with r varying) and the dashed line corresponds to $r = 10$ (with a varying). The center panel shows the conductivity for the 2×2 Dirac (solid line) and p-wave superconductor (dashed line) models as a function of the center of Q_Y. As expected, we get $-1, -2$ when the filter selects the increasing domain wall and $1, 2$ when the filter selects the decreasing domain wall, with a sharp transition in between. The right panel plots the conductivity for the 3×3 model as a function of perturbation strength, for perturbations in four distinct matrix elements. The conductivity is stable with respect to perturbations of the other five matrix elements; see text.

where

$$Q_{\Delta_\Theta}(\theta) = \begin{cases} 1, & \theta \in [-\frac{L_\theta}{4} - \Delta_\Theta, \frac{L_\theta}{4} - \Delta_\Theta] \\ 0, & \theta \notin (-\frac{L_\theta}{4} - \Delta_\Theta - \delta_\theta, \frac{L_\theta}{4} - \Delta_\Theta + \delta_\theta). \end{cases}$$

When $\Delta_Y = L_y/2$, Q would instead test the conductivity associated to the opposite, spurious, domain wall. As the center Δ_Y of the filter increases, we expect the numerical conductivity σ_I to shift from the conductivity of one domain wall to the that of the next domain wall. This is confirmed by the plot in Figure 4.3 (center) obtained for the 2×2 Dirac and p-wave superconductor models. Translating the center of Q in the x-direction would have the same effect, as the sign of P' on the support of Q changes when $\Delta_X = L_x/2$.

We finally carry out the above numerical simulations on the model of equatorial waves presented in section 2.3; see also [10]. The unperturbed Hamiltonian with symbol given in

(2.3.4) is

$$H_0 = (D_x, D_y, -f(y)) \cdot \Gamma, \tag{4.4.1}$$

where $\Gamma = (\gamma_1, \gamma_4, \gamma_7)$ with the γ_i denoting the (3×3) Gell-Mann matrices. The Coriolis force is given by $f(y)$, which changes signs across the equator. As shown in [10], the conductivity of such a system depends on the choice of f when $\mu = 0$ whereas the theory presented in section 2.3 shows that the conductivity equals 2 as soon as $\mu \neq 0$. For example, $2\pi\sigma_I = 1$ if $f = f_0 \operatorname{sgn}(y)$, and $2\pi\sigma_I = 2$ if $f(y) = \beta y$, with $f_0, \beta > 0$.

Moreover, it was shown in [10] that the conductivity is stable under perturbations of the form $V = \operatorname{diag}(V_{11}, 0, 0)$, but not $V = \operatorname{diag}(0, V_{22}, V_{33})$. We have verified these results numerically for $f(y)$ a smooth periodic function satisfying the same conditions as $m(y)$ and $c(y)$ above. For example, we see that if $V_0 = 5g_{L_y/4}(y)$ (where $g_\sigma(y)$ is the pdf of a Gaussian with mean zero and standard deviation σ), then $2\pi\tilde{\sigma}_I = 1.9950$ if $V = 0$, $2\pi\tilde{\sigma}_I = 1.9941$ if $V = \operatorname{diag}(V_0, 0, 0)$, $2\pi\tilde{\sigma}_I = -0.5394$ if $V = \operatorname{diag}(0, V_0, 0)$, and $2\pi\tilde{\sigma}_I = 0.1430$ if $V = \operatorname{diag}(0, 0, V_0)$. More generally, we have verified numerically that $\tilde{\sigma}_I$ is stable, as predicted by theory, under perturbations of the form $V(y)$ times any of the matrices

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & i & 0 \\ -i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & i \\ 0 & -i & 0 \end{pmatrix}, \tag{4.4.2}$$

and unstable under all other Hermitian perturbations, see Figure 4.3 (right).

Given that H is translationally invariant in x, we can approximate its continuous branches of spectrum by computing the eigenvalues of $\hat{H}[\xi] := (\xi, D_y, -f(y)) \cdot \Gamma$ as a function of

$$\xi \in \Big\{ \frac{2\pi j}{N_x} : j \in \{-\frac{N_x}{2}, -\frac{N_x}{2} + 1, \dots, \frac{N_x}{2} - 1\} \Big\},$$

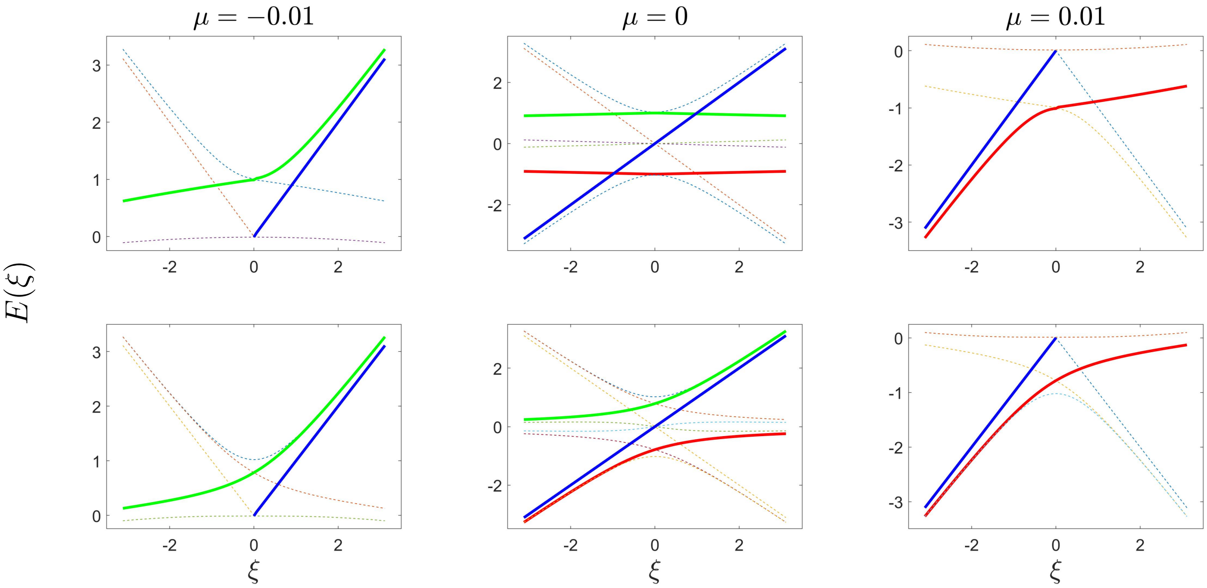

Figure 4.4: Branches of continuous spectrum for the 3×3 equatorial wave Hamiltonian, for different values of regularization parameter μ. The top line corresponds to $f(y) = \mathrm{sgn}(y)$ while the bottom line corresponds to $f(y) = \tanh(\beta y)$. The solid curves represent the nontrivial increasing branches (and the two flat bands at ± 1 when $\mu = 0$ and $f(y) = \mathrm{sgn}(y)$). For $\mu = 0$, we omit many eigenvalues approximately equal to 0, as they correspond to essential spectrum for the continuous problem. When $\mu > 0$ (resp. $\mu < 0$), these eigenvalues populate the region $\{E(\xi) > 0\}$ (resp. $\{E(\xi) < 0\}$), making it difficult to identify branches of spectrum there.

see Figure 4.4 ($\mu = 0$). Consistent with theory [10], the number of branches passing through $E = \pm 1/2$ depends on the profile of f. Namely, we obtain two nondecreasing branches of continuous spectrum passing through $E = 1/2$ when using $f(y) = \tanh(\beta y)$ and only one with $f(y) = \mathrm{sgn}(y)$. (The qualitative behavior of the branches is independent of the above perturbations under which $\tilde{\sigma_I}$ is stable.) Here, $\beta > 0$ is sufficiently small so that the transition of $f(y)$ from values near -1 to values near 1 occurs over at least several grid points. Of course, $f(y)$ is periodically wrapped, so that it in fact equals $-\tanh(\beta(y \mp L_y/2))$ in the vicinity of $y = \pm L_y/2$.

Given [10, Theorem 2.1 and Appendix B] and the fact that $\sigma_I(H) := \mathrm{Tr}\, i[H, P]\varphi'(H) = 0$ for all matrices H and P, we would expect the number of *signed* crossings of $E = 1/2$ to be 0. That is, every nondecreasing branch of spectrum passing through $E = 1/2$ should be accompanied by a nonincreasing branch that also passes through $E = 1/2$, as we observe. But these nonincreasing branches correspond to eigenfunctions that localize at $y = \pm L_y/2$ and thus become insignificant when we apply Q to compute $\tilde{\sigma}_I$.

The plots in Figure 4.4 with $\mu \neq 0$ correspond to the regularized model from Section 2.3. As expected, we find two nondecreasing branches of spectrum passing through the energy interval of interest when $f(y)$ is smooth or $\mu \neq 0$. Again, the qualitative behavior of the branches is robust to perturbations of the form (4.4.2). We see that the branches corresponding to $f(y) = \mathrm{sgn}(y)$, particularly $E(\xi) = \pm 1$ for $\mu = 0$, are more sensitive to variations in μ than those corresponding to smooth f. The flat bands are eliminated when $\mu \neq 0$, resulting in two non-trivial increasing branches of spectrum.

CHAPTER 5

INTEGRAL FORMULATION OF KLEIN-GORDON SINGULAR WAVEGUIDES

The time-harmonic Klein-Gordon equation,

$$-\Delta u + m^2 u = E^2 u$$

arises naturally in a wide variety of contexts, including condensed matter and particle physics, classical mechanics, and optics. When $|E| < m$ it models an *insulating medium*: solutions decay exponentially quickly away from a source. In the last forty years there has been particular interest in the case in which two different insulators are brought together, meeting at an interface. In such situations, depending on the physical parameters, it is possible to generate surface waves which are localized near, and propagate along, the interface.

In two dimensions, this can be modelled by the following set of partial differential equations (PDEs)

$$\begin{cases} -\Delta u(x) + m_2^2 u(x) - E^2 u(x) = f_2(x), & x \in \Omega_2, \\ -\Delta u(x) + m_1^2 u(x) - E^2 u(x) = f_1(x), & x \in \Omega_1, \\ \lim_{y \to x \in \Omega_2} u(y) = \lim_{y \to x \in \Omega_1} u(y), & x \in \Gamma, \\ \lim_{y \to x \in \Omega_2} \hat{n}(x) \cdot \nabla u(y) - \lim_{y \to x \in \Omega_1} \hat{n}(x) \cdot \nabla u(y) = -(m_1 + m_2) u(x), & x \in \Gamma, \end{cases} \tag{5.0.1}$$

where $\hat{n}(x)$ denotes the unit normal to Γ at $x \in \Gamma$ pointing in the direction of Ω_2, the domains Ω_1 and Ω_2 denote the supports of the first and second insulators, respectively, m_1 and m_2 we refer to as their 'masses', E is an energy, and f_1 and f_2 are source terms. In the sequel we will always assume that $|E|^2 < m_1^2, m_2^2$, that $\overline{\Omega_1 \cup \Omega_2} = \mathbb{R}^2$ is the entire plane, and that Ω_1 and Ω_2 meet along an interface $\Gamma = \partial\Omega_1 = \partial\Omega_2$. Moreover, we assume that Γ is a single smooth simple curve which is *asymptotically flat* in both directions and has a positive opening angle at infinity (see Section 5.1.2 for precise definitions and more detailed discussions). Intuitively, we require Γ has a smooth parameterization $\gamma : \mathbb{R} \to \Gamma$ which asymptotically approach two different rays as t goes to $-\infty$ and ∞. In order to have unique solutions, one should also supplement these equations with suitable boundary conditions at infinity and radiation boundary conditions along the interface.

In this section we construct a novel system of boundary integral equations for solving the above equation, establishing bounded invertibility for a range of masses and interfaces (see Section 5.2). Our approach is based on introducing an auxiliary variable defined via the fundamental solution of a certain time-harmonic wave equation on the interface Γ. This formulation easily lends itself to implementation. In Section 5.3 we describe an algorithm based on our boundary integral equations, and in Section 5.4 present several numerical examples.

This section focuses on solving a source problem for singular Schrödinger equations with outgoing radiation conditions for an energy range $E \in (-m_0, m_0)$. A complete spectral analysis of the problem seems quite challenging. In a subsequent work, we plan to extend the current analysis of Dirac operators and more complex geometries for interfaces.

5.1 Mathematical preliminaries

5.1.1 Detailed formulation of the problem

In this section we give a more precise statement of the problem under consideration, and summarize the associated conditions on the interface. Towards that end, suppose we are given a smooth simple curve Γ separating the plane into a lower region Ω_1 and an upper region Ω_2. Let $\gamma : \mathbb{R} \to \mathbb{R}^2$ be an arclength parameterization. Moreover, with $\hat{n}(t)$ the normal vector to γ at $t \in \mathbb{R}$ pointing in the direction of Ω_2 (using the same notation $\hat{n}$ for $\hat{n}(t)$ and $\hat{n}(\gamma(t))$ to simplify), we assume that $(\gamma'(t), \hat{n}(t))$ has positive orientation. For concreteness, we additionally assume that:

$$|\gamma'(t)| = 1, \qquad |\gamma''(t)|^2 + |\gamma'''(t)| \leq C_0 e^{-\beta|t|}\,, \tag{5.1.1}$$

$$\lim_{t\to\infty} |\gamma(\pm t)| = \infty, \qquad \lim_{t\to\infty} |\gamma(t) - \gamma(-t)| = \infty\,, \tag{5.1.2}$$

where C_0, and β are positive real constants. The fact that γ is one-to-one (along with assumption (5.1.2) above) implies the existence of some $c > 0$ such that

$$\frac{|\gamma(t) - \gamma(s)|}{|t - s|} \geq c, \qquad s, t \in \mathbb{R}. \tag{5.1.3}$$

Given a suitably-differentiable function u, for ease of exposition we set

$$\begin{aligned} [[\hat{n} \cdot \nabla u]](t) \;&:=\; \lim_{s\to 0^+} \hat{n}(t) \cdot \nabla \left[u(\gamma(t) + s\,\hat{n}(t)) - u(\gamma(t) - s\,\hat{n}(t)) \right]\,, \\ [[u]](t) \;&:=\; \lim_{s\to 0^+} \left[u(\gamma(t) + s\,\hat{n}(t)) - u(\gamma(t) - s\,\hat{n}(t)) \right]. \end{aligned}$$

Finally, we suppose that we are given positive real numbers m_1, m_2, as well as a real number E such that $|E| < \min(m_1, m_2)$. In the following we set $\omega_j = \sqrt{m_j^2 - E^2}$.

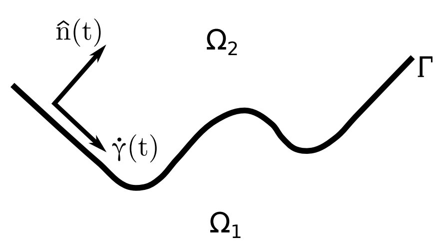

Figure 5.1: Geometry

In this paper, we consider the time-harmonic Klein Gordon equation with piecewise discontinuous masses meeting at a single one-dimensional interface:

$$\begin{aligned} -\Delta u(x) + \omega_2^2 u(x) &= f_2(x), \qquad x \in \Omega_2, \\ -\Delta u(x) + \omega_1^2 u(x) &= f_1(x), \qquad x \in \Omega_1. \end{aligned} \tag{5.1.4}$$

Here the functions f_1 and f_2 correspond to compactly-supported sources in the lower and upper regions, respectively. For ease of exposition in the following we will denote by f the function which is equal to f_2 in Ω_2 and to f_1 in Ω_1. Along the interface we enforce continuity of u as well as a jump condition in the normal derivative, as below

$$\begin{aligned} [[\hat{n} \cdot \nabla u]](\gamma(t)) &= -(m_2 + m_1) u(\gamma(t)), \qquad t \in \mathbb{R}, \\ [[u]](\gamma(t)) &= 0, \qquad t \in \mathbb{R}. \end{aligned} \tag{5.1.5}$$

Remark 5.1.1. *The continuity condition is relatively standard. The jump condition in the normal derivative is possibly less so. Our principle motivation comes from the consideration of topological insulators, as is briefly discussed in Section 5.1.2. Boundary conditions such as this also arise in the study of "leaky" waveguides, particularly in the context of "leaky quantum waveguides" (see [43] and the references therein).*

With the above assumptions, we will show that there exist solutions u of the PDE which propagate along Γ. These solutions can be interpreted as consisting in part of a surface wave emanating from the sources f_1 and f_2, confined in an exponential neighborhood of Γ. To enforce the condition that the surface wave should travel outwards (i.e. no energy should come in from infinity) we impose additional *radiation conditions*,

$$\lim_{t \to \pm\infty} (\pm \partial_t - iE) u(\gamma(t) + r\hat{n}(t)) = 0, \qquad r \neq 0, \tag{5.1.6}$$

$$\lim_{d(x,\Gamma) \to \infty} u(x) = 0, \tag{5.1.7}$$

where $d(x, \Gamma) := \min\{|x - y| : y \in \Gamma\}$ is the distance between x and Γ. The requirement

(5.1.6) is known as an *outgoing radiation condition*, and intuitively means that $u(\gamma(t)+r\hat{n}(t))$ ought to look like $Ce^{iE|t|}$ when $|t|$ is large (where $C \in \mathbb{R}$ is some constant). The outward propagation of u can be seen from the corresponding solution of the Schrödinger equation, which is of the form $e^{iE(|t|-s)}$, where s represents the time variable. Indeed, this solution is a function of $t-s$ (resp. $t+s$) when $t>0$ (resp. $t<0$). We refer to [39] for more details on this topic in similar settings.

Our main objective in this paper is the analysis of the problem (5.1.4) with boundary conditions (5.1.5, 5.1.6, 5.1.7).

5.1.2 Relation to Dirac equations and topological insulators

The above equations are closely related to certain Dirac equations arising in the study of topological insulators. In this section we elaborate on this connection in more detail. We begin by recalling that in two dimensions, the time-harmonic Dirac equation is given by

$$-i\sigma_3\partial_x\psi - i\sigma_1\partial_y\psi + m\sigma_2\psi = E\psi, \tag{5.1.8}$$

where $\psi : \mathbb{R}^2 \to \mathbb{C}^2$, $m : \mathbb{R}^2 \to \mathbb{R}$, and σ_1, σ_2, and σ_3 are the Pauli spin matrices defined by

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

Dirac equations are natural models in the description of topological insulators and the transport observed at an interface separating two insulators in different phases [17, 10, 11, 14]. In particular, if we assume that two insulators are brought together along an interface $\{y = 0\}$, we set $m(x, y) = m_2$ for $y > 0$ and $m(x, y) = -m_1$ for $y < 0$. While each region on its own acts as an insulator provided $|E| < \min(|m_1|, |m_2|) =: m_*$, this is no longer the case for the combination, which admits absolutely continuous spectra in $(-m_*, m_*)$ when the signs of

m_1 and m_2 are the same.

Squaring the Dirac equation (5.1.8) one obtains

$$-\partial_x^2\psi - \partial_y^2\psi + [m_2^2\theta(y) + m_1^2\theta(-y)]\psi - E^2\psi + (m_2 + m_1)\delta_0(y)\sigma_3\psi = 0.$$

Here $\theta(y)$ is the Heaviside function, equal to 1 for $y > 0$ and to 0 for $y \leq 0$. The above equation is diagonal, i.e. the components of ψ are not coupled. The equation for the first component is

$$-\Delta\psi_1 + [m_2^2\theta(y) + m_1^2\theta(-y)]\psi_1 - E^2\psi_1 + (m_2 + m_1)\delta_0(y)\psi_1 = 0,$$

which admits only the trivial solution $\psi_1 = 0$ (provided ψ_1 is not exponentially increasing in $|y|$). The more interesting second component satisfies

$$-\Delta\psi_2 + [m_2^2\theta(y) + m_1^2\theta(-y)]\psi_2 - E^2\psi_2 - (m_2 + m_1)\delta_0(y)\psi_2 = 0,$$

which is exactly (5.1.4, 5.1.5), at least when sources are neglected.

Our main objective in this paper is to analyze such a scalar equation and focus on the resulting propagation of signals along the interface Γ separating the insulators. In particular, we are interested in the setting where Γ is curved. The corresponding analysis to the vector-valued Dirac equation is postponed to a later study.

For an analysis of the temporal propagation of wavepackets along a curved interface in the semiclassical regime (i.e, for wavepackets asymptotically localized in the near vicinity of the interface) in both topologically trivial (Klein-Gordon) and non-trivial (Dirac) settings, see [9, 12].

5.1.3 Boundary integral operators and their properties

In this section we introduce several frequently-encountered boundary integral operators which will be useful in defining the boundary integral equations for the solution of PDE (5.1.4). We begin by recalling that for any ω in the right-half of the complex plane, the Green's function $G_\omega(x, y)$ for the PDE

$$\begin{aligned} -\Delta u(x) + \omega^2 u(x) &= \delta(x-y), \\ \lim_{|x|\to\infty} u(x) &= 0, \end{aligned} \tag{5.1.9}$$

is given by

$$G_\omega(x, y) = \frac{1}{2\pi} K_0(\omega|x-y|), \tag{5.1.10}$$

where K_0 is the modified Bessel function of the second kind.

Given a function $\rho \in L^2(\mathbb{R})$ we define its single-layer potential $S_\omega[\rho]$ by

$$S_\omega[\rho](x) = \int_{\mathbb{R}} G_\omega(x, \gamma(t))\, \rho(t)\, \mathrm{d}t$$

and its double-layer potential $D_\omega[\rho]$ by

$$D_\omega[\rho](x) = -\int_{\mathbb{R}} \hat{n}(t) \cdot \nabla_x G_\omega(x, \gamma(t))\, \rho(t)\, \mathrm{d}t$$

for $x \notin \Gamma$. Note that standard definitions of the above operators usually contain a factor of $|\gamma'(t)|$ in the integrand, while we assume that $|\gamma'| \equiv 1$. It is well-known (see [54, Lemmas 3.3 and 3.5] for example) that S_ω is continuous across Γ while D_ω and $\hat{n} \cdot \nabla S_\omega$ satisfy the following jump relations

$$\lim_{s\to 0^+} D_\omega[\rho](t \pm s\,\hat{n}(t)) = \pm\frac{1}{2}\rho(t) - \int_{\mathbb{R}} \hat{n}(t')\cdot\nabla G_\omega(\gamma(t),\gamma(t'))\,\rho(t')\,\mathrm{d}t' \tag{5.1.11}$$

$$\lim_{s\to 0^+} \hat{n}(t)\cdot\nabla S_\omega[\rho](t \pm s\,\hat{n}(t)) = \mp\frac{1}{2}\rho(t) + \int_{\mathbb{R}} \hat{n}(t)\cdot\nabla G_\omega(\gamma(t),\gamma(t'))\,\rho(t')\,\mathrm{d}t'. \tag{5.1.12}$$

We note that the two integral operators appearing on the right-hand sides of the previous equations are compact (in $L^2(\mathbb{R})$), as their kernels are continuous and rapidly decaying in t and t'. With some abuse of notation, in the following we denote these operators by $\mathcal{D}_\omega$ and $\mathcal{S}'_\omega$, respectively. We define $\mathcal{S}_\omega$ and $\mathcal{D}'_\omega$ by

$$\mathcal{S}_\omega[\rho](t) = \int_{\mathbb{R}} G_\omega(\gamma(t),\gamma(t'))\,\rho(t')\,\mathrm{d}t',$$

$$\mathcal{D}'_\omega[\rho](t) = -\int_{\mathbb{R}} \hat{n}(t')\cdot\nabla^2 G_\omega(\gamma(t),\gamma(t'))\,\hat{n}(t)\,\rho(t')\,\mathrm{d}t',$$

with $\nabla^2 G_\omega$ the Hessian of G_ω. We note that in this case, $\mathcal{S}_\omega$, $\mathcal{D}_\omega$, $\mathcal{S}'_\omega$ and $\mathcal{D}'_\omega$ can be viewed as operators from $L^2(\mathbb{R}) \to L^2(\mathbb{R})$. Finally, we remark that both $\mathcal{D}_\omega$ and $\mathcal{S}'_\omega$ are zero when restricted to any portion of the boundary which is flat. Moreover, for flat interfaces the kernels of $\mathcal{S}_\omega$ and $\mathcal{D}'_{\omega_2} - \mathcal{D}'_{\omega_1}$ have the following *Sommerfeld integral representations*

$$\mathcal{S}_\omega[\rho](t) = \int_{\mathbb{R}} K_\omega(t-t')\,\rho(t')\,\mathrm{d}t', \tag{5.1.13}$$

$$(\mathcal{D}'_{\omega_2} - \mathcal{D}'_{\omega_1})[\rho](t) = \int_{\mathbb{R}} H_{\omega_2,\omega_1}(t-t')\,\rho(t')\,\mathrm{d}t', \tag{5.1.14}$$

where

$$K_\omega(t) = \frac{1}{4\pi}\int_{\mathbb{R}} \frac{e^{i\xi t}}{\sqrt{\xi^2+\omega^2}}\mathrm{d}\xi, \tag{5.1.15}$$

$$H_{\omega_2,\omega_1}(t) = \frac{1}{4\pi}\int_{\mathbb{R}} \left(\sqrt{\xi^2+\omega_2^2} - \sqrt{\xi^2+\omega_1^2}\right) e^{i\xi t}\,\mathrm{d}\xi. \tag{5.1.16}$$

5.2 Analytical results

5.2.1 The BIEs

Let us now state the boundary integral formulation of the PDE (5.1.4, 5.1.5, 5.1.6, 5.1.7). We begin with the case $m_1 = m_2 = m$.

First, we define the operator Q via the following formula

$$Q\rho(t) = \frac{m^2}{E} \int_{\mathbb{R}} e^{iE|t-t'|} \rho(t') \mathrm{d}t', \qquad \rho \in L^2(\mathbb{R}), \tag{5.2.1}$$

and set $\mathcal{L} := 1 - 2m\mathcal{S}_\omega$ and $\mathcal{P} := 1 + Q$ so that

$$\begin{aligned} \mathcal{L}\rho(t) &= \rho(t) - 2m \int_{\mathbb{R}} G_\omega(\gamma(t), \gamma(t'))\, \rho(t')\, \mathrm{d}t', \\ \mathcal{P}\rho(t) &= \rho(t) + \frac{m^2}{E} \int_{\mathbb{R}} e^{iE|t-t'|} \rho(t') \mathrm{d}t' \,, \end{aligned} \tag{5.2.2}$$

for $\rho \in L^2(\mathbb{R})$.

Then, we seek a *density* $\rho : \mathbb{R} \to \mathbb{C}$, which satisfies the following boundary integral equation

$$\mathcal{L}\mathcal{P}\rho = 2m\, u_i, \tag{5.2.3}$$

where u_i is given by

$$u_i(x) := \int_{\mathbb{R}^2} G_\omega(x, y) f(y) \mathrm{d}y. \tag{5.2.4}$$

Here, as above, f denotes the function which is equal to f_2 in Ω_2 and f_1 in Ω_1.

The following theorem relates the solutions of (5.2.3) to the solutions of (5.1.4, 5.1.5, 5.1.6, 5.1.7).

Theorem 5.2.1. *Suppose $m_1 = m_2 =: m$. Let $\rho \in L^1$ be a solution of* (5.2.3)*, and set*

$$\mu := \mathcal{P}\rho, \qquad u_s := S_\omega[\mu], \qquad u := u_i + u_s. \tag{5.2.5}$$

Then (5.1.4)*,* (5.1.5)*,* (5.1.6) *and* (5.1.7) *hold. In particular, u constructed in this way is a solution of the PDE.*

Remark 5.2.2. *The operator Q can naturally be interpreted as the fundamental solution operator of the one-dimensional Helmholtz equation*

$$\Delta_\Gamma v + E^2 v = m^2 \rho,$$

where Δ_Γ is the Laplace-Beltrami operator of the interface curve Γ.

Remark 5.2.3. *Note that the operator Q could have equally been defined by replacing $e^{iE|t-t'|}$ by $e^{-iE|t-t'|}$. The choice of sign in* (5.2.1) *amounts to a choice of* outgoing radiation condition*, namely that we filter out incoming radiation. Indeed, if $\rho \in L^1$, then $\lim_{t\to\pm\infty}(Q\rho(t) - \frac{m^2}{E}e^{iE|t|}\hat{\rho}(\pm E)) = 0$, meaning that solutions of a time-dependent Klein Gordon problem would propagate to the right for $t > 0$ and to the left for $t < 0$ whenever $|t|$ is sufficiently large (t is the space, not time, variable here). See [39] for details on the notion of incoming and outgoing radiation.*

Suppose now that $m_1 \neq m_2$, and define $\bar{m} := \frac{1}{2}(m_1 + m_2)$. Analogous to (5.2.1), let $Q_2 : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ be given by

$$Q_2\rho(t) = \frac{\bar{m}^2}{E}\int_{\mathbb{R}} e^{iE|t-t'|}\rho(t')\mathrm{d}t', \qquad \rho \in L^2(\mathbb{R}). \tag{5.2.6}$$

We define the operator $\mathcal{L}_2 : (L^2(\mathbb{R}))^2 \to (L^2(\mathbb{R}))^2$ by

$$\mathcal{L}_2 := 1 - \begin{pmatrix} \mathcal{S}'_{\omega_2} - \mathcal{S}'_{\omega_1} + \bar{m}[\mathcal{S}_{\omega_2} + \mathcal{S}_{\omega_1}] & \bar{m}\,[\mathcal{D}_{\omega_2} + \mathcal{D}_{\omega_1}] + \mathcal{D}'_{\omega_2} - \mathcal{D}'_{\omega_1} \\ -(\mathcal{S}_{\omega_2} - \mathcal{S}_{\omega_1}) & -(\mathcal{D}_{\omega_2} - \mathcal{D}_{\omega_1}) \end{pmatrix} \tag{5.2.7}$$

and $\mathcal{P}_2 : (L^2(\mathbb{R}))^2 \to (L^2(\mathbb{R}))^2$ by

$$\mathcal{P}_2 := \left(I + V \begin{pmatrix} Q_2 & 0 \\ 0 & 0 \end{pmatrix} V^{-1} \right), \qquad V := \begin{pmatrix} -1 & \frac{1}{2m_2} - \frac{1}{2m_1} \\ \frac{1}{2m_2} - \frac{1}{2m_1} & 1 \end{pmatrix}. \tag{5.2.8}$$

Our integral equation is then to find a density $\sigma \in (L^2(\mathbb{R}))^2$ such that

$$\mathcal{L}_2 \mathcal{P}_2 \sigma = r, \tag{5.2.9}$$

where

$$\begin{aligned} r &:= \begin{pmatrix} [[\hat{n} \cdot \nabla u_i]] + 2\bar{m} u_i) \\ -[[u_i]] \end{pmatrix}, \\ u_i(x) &:= \begin{cases} \int_{\Omega_2} G_{\omega_2}(x,y) f_2(y)\, \mathrm{d}y, & x \in \Omega_2, \\ \int_{\Omega_1} G_{\omega_1}(x,y) f_1(y)\, \mathrm{d}y, & x \in \Omega_1. \end{cases} \end{aligned} \tag{5.2.10}$$

We can then relate the solutions of (5.2.9) to solutions of (5.1.4, 5.1.5, 5.1.6, 5.1.7).

Theorem 5.2.4. *Suppose $\sigma \in (L^1(\mathbb{R}))^2$ is a solution of* (5.2.9)*, and set*

$$\begin{pmatrix} \mu \\ \rho \end{pmatrix} := \mathcal{P}_2 \sigma, \qquad u_s(x) = \begin{cases} D_{\omega_2}[\rho](x) + S_{\omega_2}[\mu](x), & x \in \Omega_2, \\ D_{\omega_1}[\rho](x) + S_{\omega_1}[\mu](x), & x \in \Omega_1. \end{cases} \tag{5.2.11}$$

Then $u := u_i + u_s$ satisfies (5.1.4), (5.1.5), (5.1.6) *and* (5.1.7).

For proofs of Theorems 5.2.1 and 5.2.4, see Section 5.5.

As we will show in subsection 5.2.2 below, the integral equations (5.2.3) and (5.2.9) admit a unique solution when the interface is flat. The rest of this section concerns well-posedness of the boundary formulation for arbitrary interfaces satisfying assumptions (5.1.1) and (5.1.2). We will assume that $m_1 = m_2 =: m$ throughout. In principle, similar arguments should extend to the $m_1 \neq m_2$ case, though the presentation would be more complicated due to the presence of terms involving double layer potentials and their derivatives.

Our main results are Theorems 5.2.5 and 5.2.7 below, which state that the integral formulation (5.2.3) is well posed for "almost all" choices of m and E. The rapid decay of the curvature of γ at infinity allows for tools from perturbation theory to be applied. To prove Theorem 5.2.5, we will compare the generic (curved-interface) integral operators with their flat-interface simplifications, and show that the operator norm of the difference is small in some asymptotic regime. The difference operator also plays a central role in the proof of Theorem 5.2.7, though a smallness condition is no longer required. To distinguish between the arbitrary and flat cases, let $\mathcal{L}_0 : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ be defined by

$$\mathcal{L}_0\mu(t) := \mu(t) - \frac{m}{2\pi}\int_{\mathbb{R}}\int_{\mathbb{R}} \frac{e^{i\xi(t-t')}}{\sqrt{\xi^2+\omega^2}} \mathrm{d}\xi \, \mu(t') \, \mathrm{d}t, \qquad \mu \in L^2(\mathbb{R}), \tag{5.2.12}$$

so that $\mathcal{L}_0$ is the operator $\mathcal{L}$ in (5.2.2) when the boundary is flat. Then (5.2.3) can be rewritten as $(\mathcal{L}_0\mathcal{P} + (\mathcal{L} - \mathcal{L}_0)\mathcal{P})\rho = 2mu_i$, or equivalently

$$(1+\mathcal{M})\rho = 2m(\mathcal{L}_0\mathcal{P})^{-1}u_i, \qquad \mathcal{M} := (\mathcal{L}_0\mathcal{P})^{-1}(\mathcal{L} - \mathcal{L}_0)\mathcal{P}. \tag{5.2.13}$$

Thus to prove well-posedness of the integral formulation, it suffices to show that the operator $1+\mathcal{M}$ has bounded inverse. As suggested above, one condition that would guarantee bounded invertibility is that $\mathcal{M}$ be bounded with operator norm strictly less than 1, in which case $1+\mathcal{M}$ could be inverted by the Neumann series. But although $(\mathcal{L}_0\mathcal{P})^{-1}$ is bounded on L^2 and $\mathcal{L} - \mathcal{L}_0$ has a rapidly decaying kernel, $\mathcal{M}$ is not bounded on L^2 due to its right-most factor of $\mathcal{P}$. We thus introduce the following weighted L^2 spaces on which $\mathcal{M}$ is not only bounded but compact (to be proved in Section 5.5; see Lemma 5.5.3). For $\alpha \in \mathbb{R}$, define $w_\alpha(t) := e^{\alpha|t|}$ and $L^2_\alpha := \{\rho \in L^2(\mathbb{R}) : w_\alpha \rho \in L^2(\mathbb{R})\}$. Define $\|\cdot\|_{L^2_\alpha}$ by $\|\rho\|_{L^2_\alpha} := \|w_\alpha \rho\|_{L^2}$.

For the following, fix $m_0 > 0$ and $E_0 \in (-m_0, m_0) \setminus \{0\}$, define $\omega_0 := \sqrt{m_0^2 - E_0^2}$, and set $m = \lambda m_0$ and $E = \lambda E_0$ for $\lambda \in \mathbb{R}$. Let $\alpha_* > 0$ such that $w_{\alpha_*}(\cdot) K_0(\omega_0 |\cdot|) \in L^1$,

$$\int_{\mathbb{R}^2} \left(e^{\alpha_* t} e^{\alpha_* s} |t-s|^3 e^{-\beta \chi(s,t)} K_1(c\omega_0 |t-s|) \right)^2 \mathrm{d}t\mathrm{d}s < \infty, \qquad \alpha_* < \sqrt{\frac{\sqrt{4m_0^4 + E_0^4} - E_0^2}{2}},$$

$|\cdot|^3 K_1(c|\cdot|) \leq C e^{-\alpha_* |\cdot|}$ for some $C > 0$, and $\alpha_* < \beta$, where β and c are defined by (5.1.1) and (5.1.3), and

$$\chi(s,t) := \begin{cases} \min\{|s|, |t|\}, & st > 0 \\ 0, & \text{else.} \end{cases}$$

Here, the $K_j : (0,\infty) \to (0,\infty)$ are modified Bessel functions of the second kind. They are continuous, exponentially decaying at infinity, and satisfy $K_0(r) \sim -\log r$ and $K_1(r) \sim 1/r$ as $r \downarrow 0$. Thus α_* is indeed well defined.

We now state our first well-posedness result. Its proof uses that $\mathcal{M}$ is small in operator norm for all λ sufficiently large; see Section 5.5. Most of the theory from the proof would hold also on spaces with algebraic weights. However, the final step requires holomorphic continuation of λ into the complex plane. When λ (and hence E) has negative imaginary part, the kernel of Q has exponential growth away from the diagonal. Thus to ensure that Q is well defined, it is necessary to consider functions that decay exponentially at infinity.

Theorem 5.2.5. *For any $\alpha \in (0, \alpha_*]$, the integral equation* (5.2.3) *admits a unique solution $\rho \in L^2_\alpha$ for all but a finite number of $\lambda \in [1, \infty)$.*

Remark 5.2.6. *We note that the above dependence of m and E on λ is equivalent to setting*

$m = m_0$ and $E = E_0$ while changing γ by $\gamma_\lambda(t) := \lambda\gamma(t/\lambda)$. Thus increasing the value of λ can be thought of as stretching out the interface.

We conclude the section with a second well-posedness result, which (drops the above λ-dependence and) states that for any fixed $m > 0$, our integral formulation (5.2.3) has a unique solution for all but a countable number of values of $E \in (-m, m) \setminus \{0\}$, with 0 and $\pm m$ the only possible accumulation points of these undesirable E-values. The proof, which is postponed to Section 5.5, uses the compactness of $\mathcal{M}$ but does not require its operator norm to be small.

Theorem 5.2.7. *Fix $m > 0$. For any $\varepsilon > 0$ and $\alpha > 0$ sufficiently small (depending on ε), the integral equation* (5.2.3) *admits a unique solution $\rho \in L^2_\alpha$ for all but a finite number of $E \in [-m + \varepsilon, -\varepsilon] \cup [\varepsilon, m - \varepsilon]$.*

5.2.2 Intuitive derivation of the boundary integral equations

In this section we outline an intuitive derivation of the boundary integral equations, and sketch a proof of invertibility for the case of a flat interface. As before, we begin with the case $m_1 = m_2$.

For equal masses, the equations (5.1.4) are

$$\Delta u(x) - \omega^2 u(x) = f(x), \quad x \in \mathbb{R}^2 \setminus \Gamma, \tag{5.2.14}$$

where $\omega := \omega_1 = \omega_2$.

Then if we define the functions u_i and u_s by

$$u_i(x) := \int_{\mathbb{R}^2} G_\omega(x, y) f(y) dy, \qquad u_s := u - u_i, \tag{5.2.15}$$

and assume the existence of a *density* $\mu \in L^2(\mathbb{R})$ such that $u_s(x) = S_\omega[\mu](x)$ for all $x \in \mathbb{R}^2 \setminus \Gamma$, it follows that

$$-\mu(t) + 2m\mathcal{S}_\omega[\mu](t) = -2mu_i(\gamma(t)), \quad t \in \mathbb{R}. \tag{5.2.16}$$

Indeed, u_i is smooth across Γ and hence the definition of u_s implies

$$\begin{cases} \Delta u_s(x) - \omega^2 u_s(x) = 0, & x \in \mathbb{R}^2 \setminus \Gamma, \\ [[\hat{n} \cdot \nabla u_s]] + 2mu_s = -2mu_i, & x \in \Gamma, \end{cases} \tag{5.2.17}$$

with the added condition that $u_s + u_i$ is continuous across Γ. It is clear that the first line of (5.2.17) holds for any choice of μ, while the boundary equation (5.2.16) is a consequence of the second line of (5.2.17) together with (5.1.12) and the definition of μ.

We recognize the left-hand side of (5.2.16) as $-\mathcal{L}\mu$, where we recall the definition of $\mathcal{L}$ in (5.2.2). We will see below that for the flat-interface case, $\mathcal{L}$ has a continuous spectrum which passes through zero. As such, in general the solution will not be unique without imposing additional conditions. Moreover, if the domain is truncated, the resulting truncated operator will at best be poorly-conditioned in the limit as the length of the boundary tends to infinity and in general will not converge as the size of the truncated domain grows. For a flat interface, the problem is easily analyzed in the Fourier domain. Indeed, observing that

$$\mathcal{F}_{t\to\xi}\Big\{\frac{1}{E}e^{iE|t|}\Big\} = \lim_{\varepsilon\downarrow 0}\mathcal{F}_{t\to\xi}\Big\{\frac{1}{E+i\varepsilon}e^{i(E+i\varepsilon)|t|}\Big\} = -\frac{2i}{\xi^2 - E^2}, \tag{5.2.18}$$

we see that

$$\mathcal{F}\{\mathcal{L}\mathcal{P}\rho\}(\xi) = \Big(1 - \frac{m}{\sqrt{\xi^2+\omega^2}}\Big)\Big(1 - \frac{2im^2}{\xi^2 - E^2}\Big)\tilde{\rho}(\xi) =: a(\xi)\tilde{\rho}(\xi), \tag{5.2.19}$$

where $\mathcal{P}$ is defined in (5.2.2) and $\tilde{\rho}$ denotes the Fourier transform of ρ. Here, we used (5.1.15) to derive the Fourier representation of $\mathcal{L}$. The fact that $\mathcal{L}\mathcal{P}$ is a point-wise multiplication in the Fourier domain follows immediately from translation invariance of $\mathcal{L}$ and $\mathcal{P}$ (both kernels $k(t,t')$ are functions of only $t-t'$). The singularities of the second factor of a at $\xi = \pm E$ are canceled by the zeros of the first factor, making a an analytic function. Since a is nonzero for all ξ and converges to 1 as $|\xi| \to \infty$, there exist constants $0 < c < C$ such that $c \leq |a| \leq C$ uniformly in ξ.

We conclude that the operator $(\mathcal{LP})^{-1}$ is bounded on $L^2(\mathbb{R})$ with (bounded and analytic) Fourier symbol

$$a^{-1} = \left[\left(1 - \frac{m}{\sqrt{\xi^2+\omega^2}}\right)\left(1 - \frac{2im^2}{\xi^2 - E^2}\right)\right]^{-1} = \left(1 + \frac{m}{\sqrt{\xi^2+\omega^2}}\right)\left(1 + \frac{(2i+1)m^2}{\xi^2 - E^2 - 2im^2}\right). \tag{5.2.20}$$

This means there exists a unique function $\rho \in L^2(\mathbb{R})$ such that $\mathcal{LP}\rho = 2mu_i$, and hence the boundary integral equation is invertible (with a bounded solution).

Suppose now $m_1 \neq m_2$. This case is slightly more complicated, though the reasoning is similar to the previous case. Define the functions u_i and u_s by

$$u_i(x) = \begin{cases} \int_{\Omega_2} G_{\omega_2}(x,y) f_2(y)\,\mathrm{d}y, & x \in \Omega_2, \\ \int_{\Omega_1} G_{\omega_1}(x,y) f_1(y)\,\mathrm{d}y, & x \in \Omega_1, \end{cases} \qquad u_s := u - u_i. \tag{5.2.21}$$

Note that u_i is no longer continuous across Γ. For notational convenience, on the boundary between Ω_1 and Ω_2 we set u_i to be the average of the limits from above and below. If there are densities $\mu, \rho \in L^2(\mathbb{R})$ such that

$$u_s(x) = \begin{cases} D_{\omega_2}[\rho](x) + S_{\omega_2}[\mu](x), & x \in \Omega_2, \\ D_{\omega_1}[\rho](x) + S_{\omega_1}[\mu](x), & x \in \Omega_1, \end{cases} \tag{5.2.22}$$

then we eventually arrive at the following linear system of equations for μ and ρ,

$$\rho(t) + \left[\mathcal{D}_{\omega_2}[\rho](t) - \mathcal{D}_{\omega_1}[\rho](t)\right] + \left[\mathcal{S}_{\omega_2}[\mu](t) - \mathcal{S}_{\omega_1}[\mu](t)\right] = -\,[[u_i]](\gamma(t)), \tag{5.2.23}$$

$$\begin{aligned}-\mu(t) + \left[\mathcal{S}'_{\omega_2}[\mu](t) - \mathcal{S}'_{\omega_1}[\mu](t)\right] + \left[\mathcal{D}'_{\omega_2}[\rho](t) - \mathcal{D}'_{\omega_1}[\rho](t)\right] \\ + \bar{m}\left[\mathcal{S}_{\omega_2}[\mu](t) + \mathcal{S}_{\omega_1}[\mu](t)\right] + \bar{m}\left[\mathcal{D}_{\omega_2}[\rho](t) + \mathcal{D}_{\omega_1}[\rho](t)\right] \\ + 2\bar{m}u_i(\gamma(t)) = -\,[[\hat{n}\cdot\nabla u_i]](\gamma(t)),\end{aligned} \tag{5.2.24}$$

which are understood to hold for all $t \in \mathbb{R}$. Recall the definition $\bar{m} := \frac{1}{2}(m_1 + m_2)$. To derive the above, observe that the definition of the scattered field u_s implies that

$$\begin{cases} \Delta u_s(x) - \omega_2^2 u_s(x) = 0, \quad x \in \Omega_2, \\ \Delta u_s(x) - \omega_1^2 u_s(x) = 0, \quad x \in \Omega_1, \\ [[\hat{n}\cdot\nabla u_s]] + (m_2+m_1)u_s = -\,[[\hat{n}\cdot\nabla u_i]] - (m_2+m_1)u_i, \quad x \in \Gamma, \end{cases} \tag{5.2.25}$$

with $u_s + u_i$ continuous across Γ as before. The first two lines of (5.2.25) hold for any choice of μ and ρ. Enforcing continuity of u at the interface, and using the jump relations (5.1.11, 5.1.12) for the layer potentials, we obtain (5.2.23). Since u on Γ takes the form

$$u(\gamma(t)) = \frac{1}{2}\left[\mathcal{D}_{\omega_2}[\rho](t) + \mathcal{D}_{\omega_1}[\rho](t)\right] + \frac{1}{2}\left[\mathcal{S}_{\omega_2}[\mu](t) + \mathcal{S}_{\omega_1}[\mu](t)\right] + u_i(\gamma(t)), \tag{5.2.26}$$

the derivative jump condition in (5.2.25) implies (5.2.24).

Observe that (5.2.23, 5.2.24) reads

$$\mathcal{L}_2 \begin{pmatrix} \mu \\ \rho \end{pmatrix} = r, \tag{5.2.27}$$

where $\mathcal{L}_2$ and r are defined in (5.2.7) and (5.2.10), respectively. As above, $\mathcal{L}_2$ may admit a continuous spectrum passing through zero, hence solving for (μ, ρ) in (5.2.27) is in general an ill-posed problem.

To remedy this issue, we again turn our attention to the special case of a flat boundary, where Fourier representations of the relevant integral operators are given by (5.1.15) and (5.1.16). Taking the Fourier transform of (5.2.23) in the flat case, we find that

$$\tilde{\rho}(\xi) + \frac{1}{2}\left[\frac{1}{\sqrt{\xi^2+\omega_2^2}} - \frac{1}{\sqrt{\xi^2+\omega_1^2}}\right]\tilde{\mu}(\xi) = -\left[\left[\tilde{u}_i\right]\right](\xi). \tag{5.2.28}$$

Similarly, upon taking the Fourier transform of (5.2.24), we obtain

$$\begin{aligned} -\tilde{\mu} - \frac{1}{2}\left[\sqrt{\xi^2+\omega_2^2} - \sqrt{\xi^2+\omega_1^2}\right]\tilde{\rho} + \frac{m_2+m_1}{4}\left[\frac{1}{\sqrt{\xi^2+\omega_2^2}} + \frac{1}{\sqrt{\xi^2+\omega_1^2}}\right]\tilde{\mu} \\ = -\frac{m_2+m_1}{2}(\tilde{u}_{i,1}+\tilde{u}_{i,2}) - \left[\left[\widetilde{\hat{n}\cdot\nabla u_i}\right]\right]. \end{aligned} \tag{5.2.29}$$

After solving (5.2.28) for $\tilde{\rho}$ and substituting it into (5.2.29) we see that

$$\left[-1 + \frac{1}{4}(\xi_2-\xi_1)(\xi_2^{-1}-\xi_1^{-1}) + \frac{m_2+m_1}{4}(\xi_2^{-1}+\xi_1^{-1})\right]\tilde{\mu} = \tilde{\psi} \tag{5.2.30}$$

where $\xi_{1,2} = \sqrt{\xi^2+\omega_{1,2}^2} = \sqrt{\xi^2+m_{1,2}^2-E^2}$, and

$$\tilde{\psi}(\xi) = -\frac{m_2+m_1}{2}(\tilde{u}_{i,1}+\tilde{u}_{i,2}) - \left[\left[\widetilde{\hat{n}\cdot\nabla u_i}\right]\right] - \frac{1}{2}(\xi_2-\xi_1)\left[\left[\tilde{u}_i\right]\right](\xi).$$

Let $R(\xi)$ denote the Fourier multiplier from the left-hand side of (5.2.30) defined by

$$R(\xi) := -1 + \frac{1}{4}(\xi_2-\xi_1)(\xi_2^{-1}-\xi_1^{-1}) + \frac{m_2+m_1}{4}(\xi_2^{-1}+\xi_1^{-1}). \tag{5.2.31}$$

Differentiating (5.2.31) with respect to ξ^2 we see that

$$\frac{\mathrm{d}}{\mathrm{d}\xi^2}R(\xi) = -\frac{m_2+m_1}{8}\frac{\xi_2^3+\xi_1^3}{\xi_1^3\xi_2^3} + \frac{1}{8}\frac{(\xi_2^2-\xi_1^2)^2}{\xi_1^3\xi_2^3}.$$

Now, $\xi_2^2 - \xi_1^2 = \omega_2^2 - \omega_1^2$, $\xi_2 \geq \omega_2$, $\xi_1 \geq \omega_1$, and $m_1 + m_2 > \omega_1 + \omega_2$, from which it follows that

$$(m_2+m_1)(\xi_2^3+\xi_1^3) - (\xi_2^2-\xi_1^2)^2 \geq \omega_2^4 + \omega_1^4 - \omega_2^4 - \omega_1^4 + 2\omega_2^2\omega_1^2 > 0.$$

In particular, $R(\xi)$ is decreasing for $\xi < 0$ and increasing for $\xi > 0$, from which it follows immediately that $\xi = \pm E$ are the only roots.

Finally, we observe that the nullvectors $(\tilde{\mu}(\xi), \tilde{\rho}(\xi))^t$ associated with $\xi = \pm E$ are both

$$v = \begin{pmatrix} -1 \\ \frac{1}{2m_2} - \frac{1}{2m_1} \end{pmatrix}. \tag{5.2.32}$$

Motivated by this, we change variables to remove the singularity captured by the nullvectors in (5.2.32). Namely, we introduce the new unknowns, σ_1 and σ_2 defined implicitly by

$$\begin{pmatrix} \mu \\ \rho \end{pmatrix} = \mathcal{P}_2 \begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix}, \tag{5.2.33}$$

with $\mathcal{P}_2$ given by (5.2.8). As with Q for the one-mass case, the Fourier transform of Q_2 has singularities at $\xi = \pm E$. Thus the singularities of $\mathcal{P}_2$ exactly cancel the zeros of $\mathcal{L}_2$. Substituting (5.2.33) into the Fourier transformed boundary integral equations (5.2.28) and (5.2.29), we obtain an invertible system for σ_1 and σ_2. In particular, $\mathcal{L}_2\mathcal{P}_2$ is bounded with bounded inverse.

5.3 Numerical apparatus

In this section we describe an algorithm for solving equations (5.1.4, 5.1.6, 5.1.7) via the boundary integral equations (5.2.3) and (5.2.5). For notational convenience we present only the case in which $m_1 = m_2 =: m$. The more general case can be solved in a similar way. In subsection 5.3.1 we briefly discuss the details of the discretization used. Following this, in subsection 5.3.2 we describe several accelerations that were made to improve the computational efficiency.

5.3.1 The discretization

In this section, we use the boundary integral equation package `chunkie` (see [27]) to discretize the interface and construct the entries of the discrete approximation to the operators $\mathcal{L}$ and $\mathcal{P}$ given by (5.2.2) and $\mathcal{L}_2$ and $\mathcal{P}_2$ defined in (5.2.7) and (5.2.8). To simplify the presentation of our method, we assume that $m_1 = m_2 =: m$ throughout this section. This means the relevant integral equation is $\mathcal{L}\mathcal{P}\rho = 2mu_i$.

The interface is truncated to $[a, b]$ in parameter space, i.e. we restrict $\gamma(t) : [a, b]$ to its image. This truncated curve is then adaptively split into "chunks" where each chunk is the image of a subinterval of $[a, b]$, and is discretized using 16 Gauss-Legendre points. Chunks are refined until the tails of the Legendre coefficients of the speed of parameterization, and of the x, y coordinates of the curve are resolved. In particular, suppose that $x_n^{(j)}, y_n^{(j)}, s_n^{(j)}$ are the the Legendre coefficients computed using 32 nodes on a chunk $[a_j, b_j]$, i.e.

$$\begin{bmatrix} x(t) \\ y(t) \\ s(t) \end{bmatrix} = \sum_{n=1}^{32} \begin{bmatrix} x_n^{(j)} \\ y_n^{(j)} \\ s_n^{(j)} \end{bmatrix} P_n\left(a_j + \frac{(t+1)}{2}(b_j - a_j)\right), \tag{5.3.1}$$

where $s(t) = |\gamma'(t)|$, and $P_n(t)$ is the Legendre polynomial of degree n on $[-1, 1]$. Then the chunk $[a_j, b_j]$ is resolved if

$$\max\left(\sqrt{\frac{\sum_{n=17}^{32}|x_n|^2}{16}}, \sqrt{\frac{\sum_{n=17}^{32}|y_n|^2}{16}}, \sqrt{\frac{\sum_{n=17}^{32}|s_n|^2}{16}}\right) \leq \varepsilon\,, \tag{5.3.2}$$

for a specified tolerance ε. If the chunk is not resolved, then it is split into two chunks of equal length in parameter space $[a_j, (a_j+b_j)/2]$, and $[(a_j+b_j)/2, b_j]$. Once all of the chunks are resolved, they are subsequently balanced so that adjacent chunks satisfy a $2:1$ length restriction: if γ_j and γ_ℓ are adjacent to each other then they satisfy $|\gamma_j|/|\gamma_\ell| \in [0.5, 2]$. At the end of the adaptive procedure, the restriction of γ to $[a, b]$ is represented via a collection of n_c chunks, $[a, b] = \cup_{j=1}^{n_c}[a_j, a_{j+1}]$ with the understanding that $a_1 = a$, and $a_{n_c+1} = b$.

Remark 5.3.1. *In the proofs, we have assumed $\gamma' \equiv 1$ for convenience. The proofs can be suitably modified as long as $||\gamma'| - 1| \leq Ce^{-\alpha|t|}$ for some positive constants C and α. Relaxing this restriction provides greater flexibility for parametrizing complicated curves.*

Recall that the solution $\rho \in L^2_\alpha(\mathbb{R})$, and hence there exists an M such that

$$\sqrt{\frac{\int_{[-\infty,-M]\cup[M,\infty]}|\rho|^2\,ds}{\int_{-\infty}^{\infty}|\rho|^2\,ds}} \leq \varepsilon\,. \tag{5.3.3}$$

This estimate justifies the existence of a truncation $[a, b]$ such that the solution can be accurately represented via its restriction to some bounded interval of $\mathbb{R}$. In all the examples, the interval $[a, b]$ is taken to be the smallest interval satisfying the following two criteria: a) that the boundary is nearly flat outside of $[a, b]$, i.e. there exists a constant vector $c \in \mathbb{R}^2$, such that $|\gamma'(t) - c| \leq \varepsilon$ for all $c \in \mathbb{R}^2 \setminus [a, b]$, and b) the boundary data u_i is numerically supported on $[a, b]$ to precision ε, i.e. $|u_i|_{L^2(\mathbb{R}\setminus[a,b])}/|u_i|_{L^2(\mathbb{R})} \leq \varepsilon$.

Given these restrictions, the composition $\mathcal{LP}$ is discretized as an intergral operator on L^2 functions defined on the interval $[a, b]$. Even though ρ will be numerically supported on $[a, b]$, the operator $\mathcal{P}$ maps compactly supported functions to an oscillatory function that is

$O(1)$ on the whole real line. On the other hand, the kernel in the integral operator $\mathcal{L}$ decays exponentially as $\exp(-\omega d)$, where d denotes the Euclidean distance between points on the interface. Thus, in order to compute the solution ρ accurately, one needs to discretize the integral operator $\mathcal{P}$ from L^2 functions on $[a, b]$ to L^2 functions on $[a', b']$, and the integral operator $\mathcal{L}$ from L^2 functions on $[a', b']$ to L^2 functions $[a, b]$, where $a' = a - \log(1/\varepsilon)/\omega$, and $b' = b + \log(1/\varepsilon)/\omega$. The necessity and sufficiency of this choice of the buffer region is illustrated through the results in Section 5.4.1.

We now turn our attention to the discretization of the integral operators $\mathcal{L}$ and $\mathcal{P}$. Suppose that there are an additional n_{buffer} points introduced in each of the buffer regions $[a', a]$ and $[b, b']$. Suppose that $t_j \in [a', b']$, $j = 1, 2 \ldots n_{\text{over}} = 16n_c + 2n_{\text{buffer}}$ are the discretized values of t in parameter space. Let $n_0 = n_{\text{buffer}} + 16n_c$. Suppose that the points are ordered in increasing values of t. Then the points $j = 1, 2 \ldots n_{\text{buffer}}$ correspond to the left buffer region $[a', a]$, the points $j = n_{\text{buffer}} + 1, \ldots n_0$ correspond to the interval $[a, b]$, and the points $j = n_0 + 1, \ldots n_{\text{over}}$ correspond to the right buffer region $[b, b']$. Note that the density ρ is discretized through its values at $\rho(t_j)$, for $j = n_{\text{buffer}} + 1, \ldots n_0$, and hence the discretized linear system corresponding to $\mathcal{LP}$ will be of size $n_0 - n_{\text{buffer}} = 16n_c$.

Both the kernels $\mathcal{L}$ and $\mathcal{P}$ have non-smooth and at most weakly singular kernels for small distances and require specialized quadrature rules for integrating them. We use the generalized Gaussian quadrature rules of [22, 21] for the accurate computation of these integrals. In particular, the quadrature rule is a target dependent locally-corrected quadrature rule which accurately integrates the specific non-smooth behavior of the kernel in the vicinity of the origin. For every point $t_j \in [a_i, a_{i+1}]$, there exist weights $w_{j,\ell}$ for all $t_\ell \in [a_{i-1}, a_{i+1}]$ such that the discretized versions of $\mathcal{P}$ and $\mathcal{L}$, denoted by $\mathbf{P}$ and $\mathbf{L}$ respectively, are given by

$$
\begin{aligned}
\mathbf{P}[\rho](t_j) = \frac{m^2}{E} & \sum_{\ell=n_{\text{buffer}}+1}^{n_0} (\delta_{j,\ell} + e^{iE|t_j - t_\ell|} w_\ell)\rho(t_\ell) \\
& + \sum_{\substack{\ell=n_{\text{buffer}}+1 \\ t_\ell \in [a_{i-1}, a_{i+1}]}}^{n_0} \rho(t_\ell) w_{j,\ell}\,, \quad j = 1, 2, \ldots n_{\text{over}} \\
\mathbf{L}[\mu](t_j) = \mu(t_j) - 2m & \sum_{\substack{\ell=1 \\ \ell \neq j}}^{n_{\text{over}}} G_\omega(\gamma(t_j), \gamma(t_\ell))\mu(t_\ell) w_\ell \\
& + \sum_{\substack{\ell=1 \\ t_\ell \in [a_{i-1}, a_{i+1}]}}^{n_{\text{over}}} \mu(t_\ell) w_{j,\ell}\,, \quad j = n_{\text{buffer}} + 1, n_{\text{buffer}} + 2, \ldots n_0\,.
\end{aligned}
\tag{5.3.4}
$$

Here $\delta_{j,\ell}$ is the Kronecker delta, i.e. $\delta_{j,j} = 1$ and $\delta_{j,\ell} = 0$ otherwise, and w_j, $j = 1, 2 \ldots n_{\text{over}}$, denote the quadrature weights for integrating smooth functions on the interface. The factorized linear systems $\mathbf{L}$ and $\mathbf{P}$ are illustrated in Figure 5.3.

Remark 5.3.2. *Recall that $\mathcal{L}$ may have a continuous spectrum passing through zero while $\mathcal{P}$ is not bounded; see* (5.2.19)*. Thus it is expected (and observed numerically) that in general, $\mathbf{L}$ and $\mathbf{P}$ both have very large condition numbers. This could in principle lead to catastrophic cancellation arising from the numerical implementation of the operator product $\mathbf{LP}$. We postpone a thorough treatment of this potential issue to future study. Practically speaking, the accuracy of our numerical method does not seem to suffer from the poor condition numbers of $\mathbf{L}$ and $\mathbf{P}$. Indeed, as illustrated by Section 5.4.1, we observe low errors for a variety of interfaces and wide range of parameters.*

5.3.2 Accelerations of the numerical method

In this section, we discuss a fast algorithm for the evaluation of the matrix vector product $\mathbf{LP}[\rho]$. The kernel of $\mathbf{P}$ is the Green's function of a one-dimensional translation-invariant el-

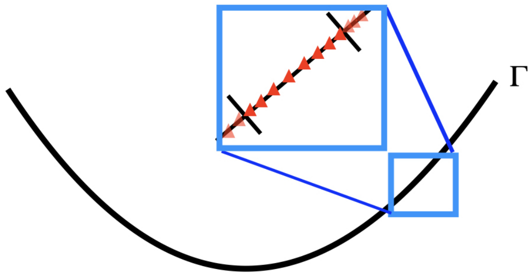

Figure 5.2: Schematic of the discretization approach used by `chunkie`. In the inlay, bounds between 'chunks' are shown with vertical lines, and discretization nodes are denoted by red triangles. For clarity, the 'panel' shown is 8^{th} rather than 16^{th}.

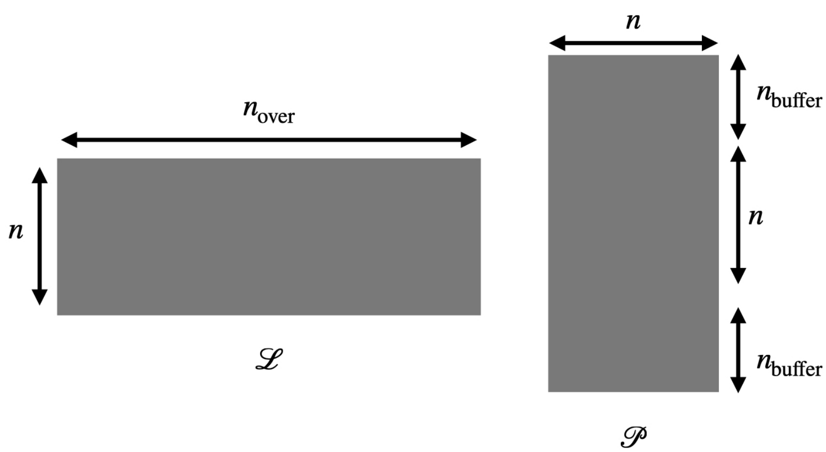

Figure 5.3: The factorized linear system, after discretization.

liptic ordinary differential equation and hence can be accelerated using a sweeping algorithm. In order to apply P rapidly, we just need a fast algorithm for the evaluation of

$$\mathsf{P}[\rho](t_j) = \frac{m^2}{E} \sum_{\ell=n_{\text{buffer}}+1}^{n_0} e^{iE|t_j - t_\ell|} \rho(t_\ell) w_\ell \,, \quad j = 1, 2, \ldots n_{\text{over}} \,, \tag{5.3.5}$$

since the rest of the interaction is sparse and can be computed in $O(n_{\text{over}})$ CPU time. The main idea of the sweeping algorithm is to split the solution into two parts for any point t_j, $t \le t_j$, and $t > t_j$, where both pieces can be updated in $O(1)$ operations as we move from $t_j \to t_{j+1}$ or $t_j \to t_{j-1}$. Let $v^{\uparrow}$ and $v^{\downarrow}$ denote the accumulation of the rightward moving solution (corresponding to $t \leq t_j$) and the leftward moving solution(corresponding to $t > t_j$) respectively.

In particular, we split the solution as follows,

$$
\begin{aligned}
P[\rho](t_j) &= \frac{m^2}{E} \sum_{\substack{\ell=n_{\text{buffer}}+1 \\ \ell \leq j}}^{n_0} e^{iE(t_j - t_\ell)} \rho(t_\ell) w_\ell + \frac{m^2}{E} \sum_{\substack{\ell=n_{\text{buffer}}+1 \\ \ell > j}}^{n_0} e^{iE(t_\ell - t_j)} \rho(t_\ell) w_\ell \\
&= v_j^{\uparrow} + v_j^{\downarrow} \,.
\end{aligned}
\tag{5.3.6}
$$

A simple calculation shows that $v^{\uparrow}$ and $v^{\downarrow}$ satisfy the following recurrence relations

$$
\begin{aligned}
v_j^{\uparrow} &= v_{j-1}^{\uparrow} e^{iE(t_j - t_{j-1})} + \frac{m^2}{E} \rho(t_j) w_j I_{j \in [n_{\text{buffer}}+1, n_0]} \,, \\
v_j^{\downarrow} &= e^{iE(t_{j+1} - t_j)} \left(v_{j+1}^{\downarrow} + \frac{m^2}{E} \rho(t_{j+1}) w_{j+1} I_{j+1 \in [n_{\text{buffer}}+1, n_0]} \right) \,,
\end{aligned}
\tag{5.3.7}
$$

where $I_{j\in A}$ is the indicator function of the set A, which is equal to 1 if $j \in A$, and 0 otherwise. Thus, $v^{\uparrow}$ satisfies an upward recurrence in j, while $v^{\downarrow}$ satisfies a downward recurrence, and both $v^{\uparrow}$ and $v^{\downarrow}$ can be computed for all j in $O(n_{\text{over}})$ work. The recurrences are initialized with $v_1^{\uparrow} = 0$, and $v_{n_{\text{over}}}^{\downarrow} = 0$.

On the other hand, the kernel of $\mathbf{L}$ is the Green's function of the two dimensional Helmholtz equation with imaginary wave number ω and the bulk of the computation is given by

$$
-2m \sum_{\substack{\ell=1 \\ \ell \neq j}}^{n_{\text{over}}} G_\omega(\gamma(t_j), \gamma(t_\ell)) \mu(t_\ell) w_\ell \,, \quad j = n_{\text{buffer}} + 1, \ldots n_0 \,. \tag{5.3.8}
$$

The above sum can be computed at all t_j, $j = n_{\text{buffer}} + 1, \ldots n_0$ in $O(n_{\text{over}})$ CPU time using the standard fast multipole method; see [73, 50]. We use the fast multipole implementation in `fmm2d` for evaluating the sum in [45]. The rest of the computation in $\mathbf{L}$ is sparse whose number of nonzero elements is also $O(n_{\text{over}})$.

Combining both of these fast algorithms, the matrix vector product $\mathbf{LP}[\rho]$ can be applied in $O(n_{\text{over}})$ CPU time. Thus, the solution ρ can be obtained in $O(n_{\text{over}} n_{\text{iter}})$ CPU time using iterative methods like the generalized minimum residual (GMRES) method, where n_{iter} is the number of GMRES iterations required for the relative residual to drop below a prescribed tolerance. In practice, the integral equation tends to be well-conditioned which results in $n_{\text{iter}} = O(1)$, and thus the computational complexity of obtaining the solution ρ is $O(n_{\text{over}})$.

5.4 Numerical illustrations and examples

In this section, we provide several examples of the numerical method described in Section 5.3. We demonstrate accuracy or self-convergence of the algorithm and test its speed for a variety of interfaces; see subsection 5.4.1. In subsection 5.4.2, we plot corresponding solutions and compute reflection coefficients for a scattering theory. We refer to Figure 5.4 for an illustration of the interfaces used in our examples.

5.4.1 Illustration of the numerical method

This section presents the accuracy and speed of our numerical method for various interfaces. We begin with the flat-interface (Γ_0) case, where there is an analytic expression for the Green's function. For simplicity, we assume that $m_1 = m_2 =: m$. If u denotes our computed solution, we define the relative error of u at the point x_T by $|u(x_T) - u_*(x_T)|/|u_*(x_T)|$, where u_* is the true solution. Figure 5.5 contains a plot of this relative error (computed at four arbitrary points) as a function of n_c, as well as illustrations of the computed Green's function and densities. Observe that our solution is highly accurate even for small values of n_c.

For arbitrary non-flat interfaces (such as $\Gamma_1, \Gamma_2, \Gamma_3$), analytic solutions are not known and hence we cannot compute the exact relative error. Instead, we perform a self-convergence test, which involves approximating the true solution by the numerical solution at some

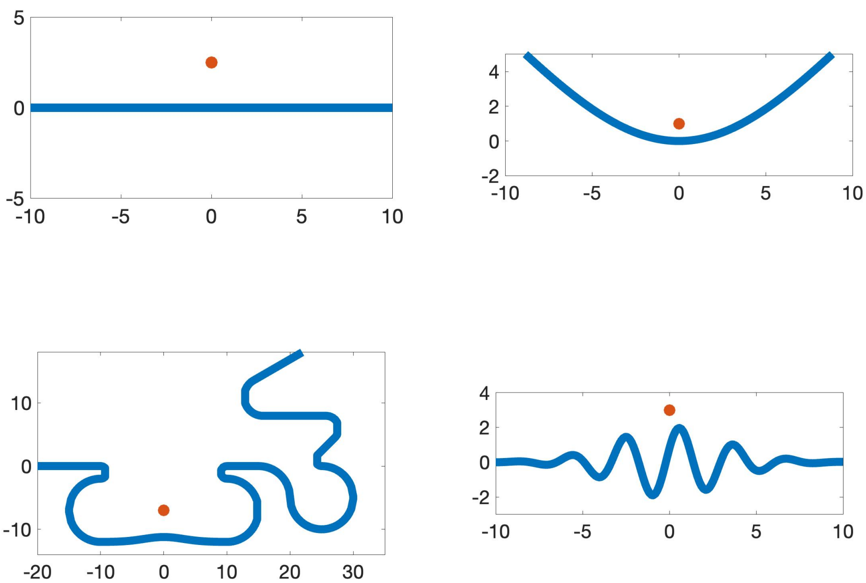

Figure 5.4: The interfaces Γ_0 (top left), Γ_1 (top right), Γ_2 (bottom left) and Γ_3 (bottom right), with respective sources at $(0, 2.5)$, $(0, 1)$, $(0, -7)$ and $(0, 3)$ as indicated by the red dot. Outside the plotted region, the interfaces extend linearly to infinity.

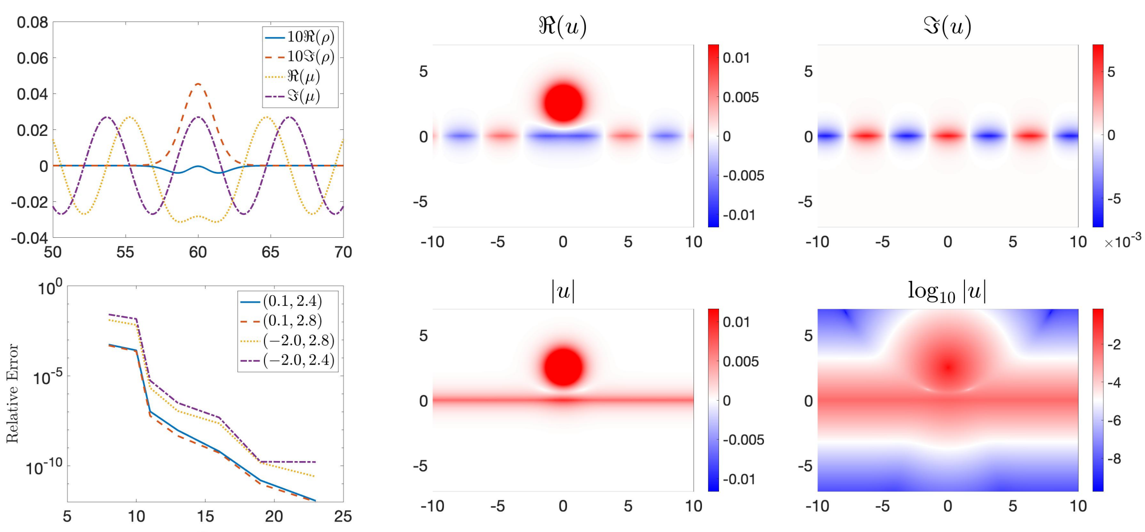

Figure 5.5: Densities μ and ρ (top left panel), relative error of the computed solution at the indicated points as a function of n_c (bottom left panel), and Green's function u (center and right panels) corresponding to the flat interface Γ_0 with $m = 2$ and $E = 1$. The top left panel zooms in on the region $[10, 10] \times \{0\} \subset \Gamma_0$, with $t = 60$ corresponding to the point $(0, 0) \in \Gamma_0$.

large value N^* of n_c. If we now let u_N denote the computed solution with $n_c = N$, our approximate relative error at the target x_T is given by $|u_N(x_T) - u_{N^*}(x_T)|/|u_{N^*}(x_T)|$. For a corresponding plot with $N^* = 512$, see Figure 5.6 (left panel). We again observe fast convergence in n_c, though understandably not as fast as the flat-interface case.

Another parameter of interest is the truncation length n_{buffer} (introduced in Section 5.3.1). Its default value (unless otherwise specified) is

$$n_{\text{buffer}} = 2\left\lceil \frac{n_c \log(10^{16})}{m_0 \Delta_t} \right\rceil =: 2\lceil M_b \rceil,$$

where $m_0 := \min(m_1, m_2)$ and Δ_t is the arclength of Γ over the entire discretized region (that is, the region discretized by all $n_{\text{over}} = n + 2n_{\text{buffer}}$ grid points; see Section 5.3.1). Here, $M_b \in \mathbb{N}$ is sufficiently large so that interactions between points separated by at least M_b grid points are bounded by 10^{-16} in absolute value. Some routines in the numerical experiments presented here were set to a tolerance of 10^{-12}, so the error of 10^{-16} more than ensures that any error we observe would not be due to truncation.

To test the effect of n_{buffer} on the convergence of our method, we introduce $\tau > 0$ and set $n_{\text{buffer}} = 2\lceil \tau M_b \rceil$. In the center panel of Figure 5.6, we plot

$$|u_{n_c,\tau}(x_T) - u_{512,\tau}(x_T)|/|u_{512,\tau}(x_T)|$$

as a function of τ, where $u_{N,\tau}$ is our computed solution with $n_c = N$ and $n_{\text{buffer}} = 2\lceil \tau M_b \rceil$. We set $n_c = 128, 64, 256$ for $\Gamma_1, \Gamma_2, \Gamma_3$, respectively. Given the small truncation error tolerance at $\tau = 1$, it makes sense that decreasing the value of τ from 1 would not immediately increase the relative error. Still, once τ gets small enough (say, less than 0.5), the truncation length is too small and the convergence of our method suffers. The relative error increases when τ increases from 1, as we do not keep enough grid points in this case.

In summary, the left panel illustrates relative error at fixed $\tau = 1$ and varying n_c, while

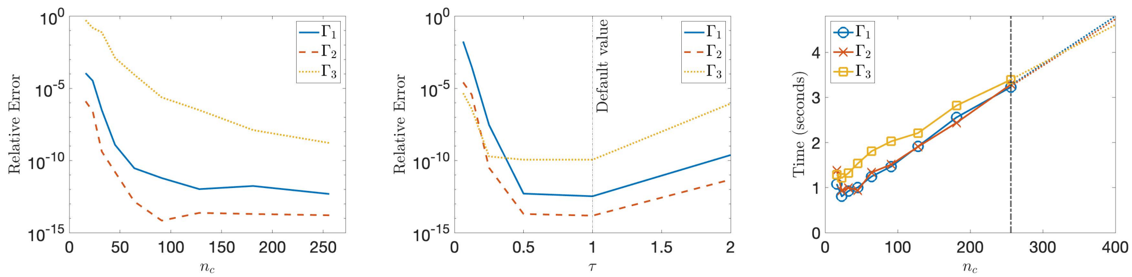

Figure 5.6: Self-convergence tests for varying n_c (left panel) and truncation length (center panel). The relative error is computed at $x_T = (-1, 1), (7, -7), (1, -3)$ for $\Gamma_1, \Gamma_2, \Gamma_3$ respectively. For each interface, the source location is given by Figure 5.4. The respective values of m and E are those from Figures 5.7 (top right panel), 5.8 and 5.9 below. The computational cost of obtaining $u(x_T)$ is illustrated by the right panel.

the center panel illustrates relative error at fixed n_c (depending on the interface) and varying τ. We refer to the right panel of Figure 5.6 for a plot of the speed of our method as a function of n_c. As predicted, the computation time grows only linearly in n_c. The respective slopes of the line of best fit for $\Gamma_1, \Gamma_2, \Gamma_3$ are $1.06 \times 10^{-2}, 1.03 \times 10^{-2}, 8.43 \times 10^{-3}$, with an average value of 9.78×10^{-3}. These slopes were computed using only the data for $n_c > 50$ to eliminate the effect of the nonlinear behavior of the curves for small n_c. The lines of best fit are used to extrapolate the data to $n_c > 256$ in the plot.

5.4.2 *Examples of applications*

We now present various examples corresponding to the non-flat interfaces from Figure 5.4. The Green's function, u, and densities, μ and ρ, for a source (whose location is given by Figure 5.4) near a non-flat section of the interface are plotted in Figures 5.7–5.10. As expected, $\omega = \sqrt{m^2 - E^2}$ dictates the rate at which solutions decay away from the interface. In particular, larger values of ω result in faster decaying solutions. In the case of different masses, we observe that u decays more rapidly in the domain with larger ω; see Figures 5.7 and 5.10.

Our numerical experiments (Figures 5.5 and 5.9) verify that the density ρ from (5.2.5) is

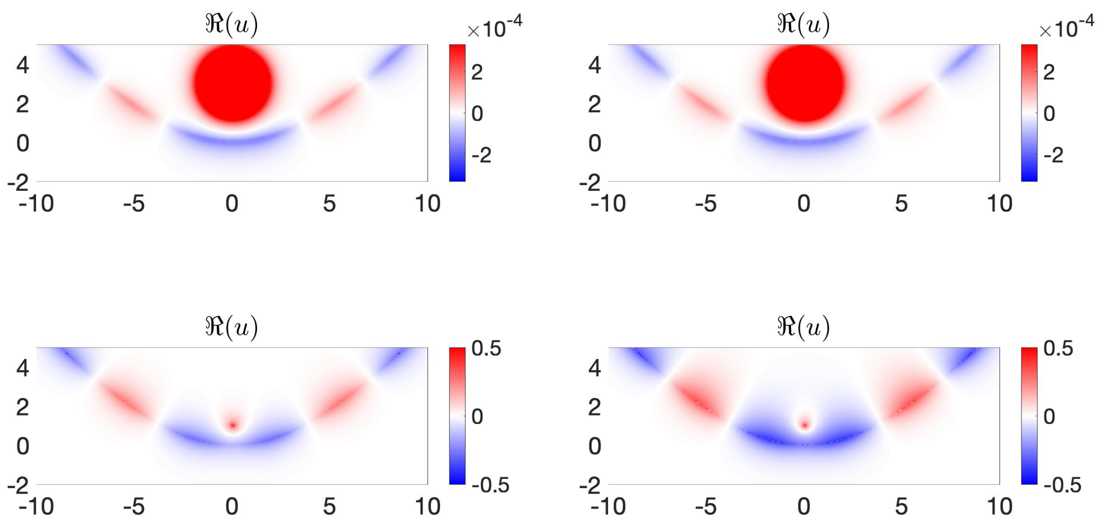

Figure 5.7: Green's function, u, for interface Γ_1 with $m_1 = 2$, $E = 0.8$ and $m_2 = 3$ (top left) $m_2 = 2$ (top right), $m_2 = 1.5$ (bottom left) and $m_2 = 1$ (bottom right).

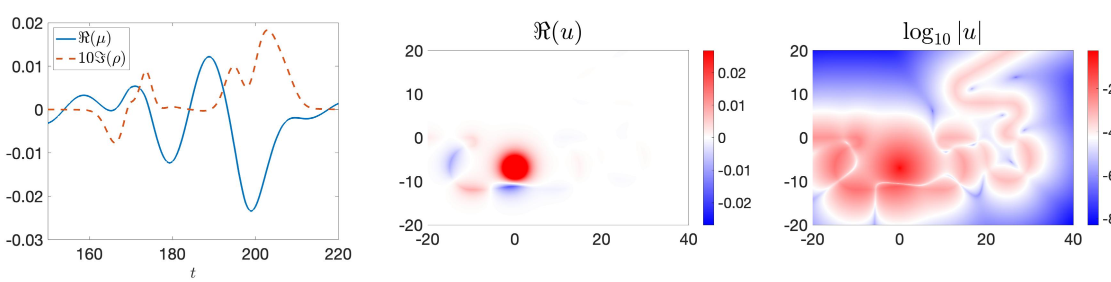

Figure 5.8: Densities, μ and ρ, and Green's function, u, for the interface Γ_2 with $m_1 = m_2 = 2/3$ and $E = 1/3$. The left plot zooms in on the part of Γ_2 connecting the points $(-30.0, 0.0)$ and $(14.8, -8.5)$, with $t = 185$ corresponding to the point $(-13.5, -10.6)$.

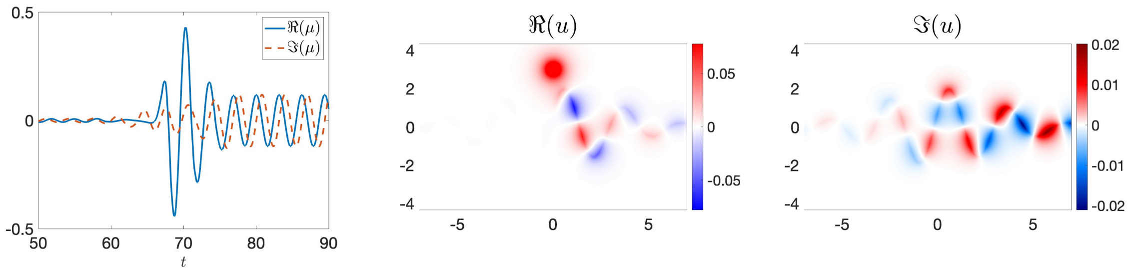

Figure 5.9: Density, μ, and Green's function, u, for the interface Γ_3 with $m_1 = m_2 = 3$ and $E = 2$. The left plot zooms in on the part of Γ_3 connecting the points $(-10.0, 0.0)$ and $(18.0, 0.0)$, with $t = 70$ corresponding to the point $(1.4, -0.2)$.

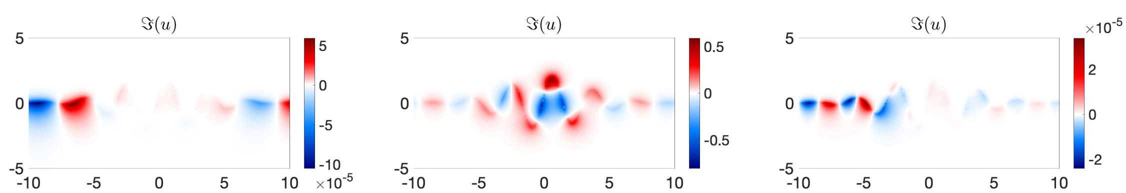

Figure 5.10: Green's function, u, for the interface Γ_3, where $(m_1, m_2, E) = (1.20, 4.00, 1.00)$ for the left panel, $(m_1, m_2, E) = (2.00, 3.00, 1.50)$ for the center panel, and $(m_1, m_2, E) = (2.25, 6.00, 2.00)$ for the right panel.

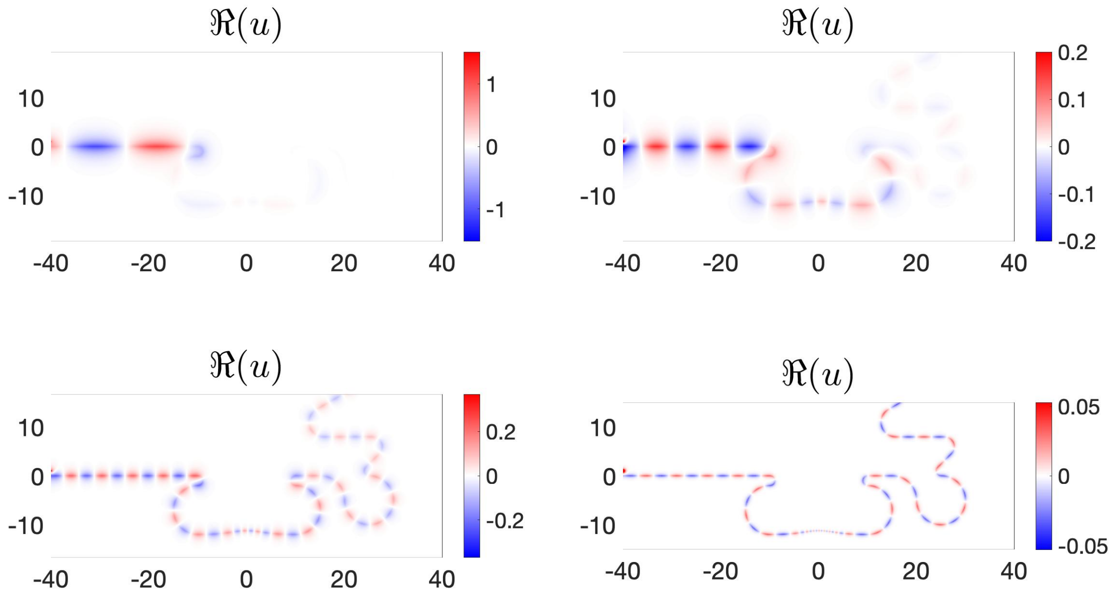

Figure 5.11: Green's function, u, for the interface Γ_2 with source located at $(-40, 1)$. Here, (m, E) is $(0.75, 0.25)$, $(0.75, 0.5)$, $(1.5, 1)$ and $(4, 1)$ for the top-left, top-right, bottom-left and bottom-right panels, respectively.

rapidly decaying, while $\mu := \mathcal{P}\rho$ obeys an outgoing radiation condition, oscillating without decay. For an illustration of ρ and μ in the vicinity of a source (zooming in on the region where ρ is not small), see Figure 5.8.

In Figure 5.11 we move the source to $(-40, 1)$ and observe that the propagation of the resulting wave along the interface depends on the choice of (m, E). As stated in Remark 5.2.6, increasing the value of ω is equivalent to smoothing out the interface, thus it makes sense that the solutions on the top row get reflected while those on the bottom get transmitted. Similarly, the small values of m and E in Figure 5.8 (combined with the corresponding source location; see Figure 5.4, bottom left panel) result in a solution that is concentrated near the oscillatory part of Γ_2.

We conclude this section with a scattering experiment. Let us consider the interface parametrized by $\gamma(t) = 2e^{-0.05t^2}\sin(bt + 0.4)$, for some $b \geq 0$. Note that the value $b = 2$ gives Γ_3. We place a source near the interface, to the left of and far away from its oscillations.

The density μ is proportional to the solution u along the interface, as (5.2.16) implies that $\mu = 2m(u_i + u_s) = 2mu$ on Γ. The outgoing condition (5.1.6) implies that $\mu(t) \approx Ce^{iEt}$ for $t > 0$ sufficiently large. Between the source and oscillations, we have that $\mu(t) \approx Ae^{iEt} + Be^{-iEt}$, where $|A|$ and $|B|$ are the respective amplitudes of the incoming and reflected waves. The transmission and reflection coefficients are then defined by $T_L := |C|^2/|A|^2$ and $R_L := |B|^2/|A|^2$.

Since $\mu = (1 + Q)\rho$ with $\rho \in L^1$, it follows that $\mu(t) \approx \frac{m^2}{E}e^{\pm iEt}\hat{\rho}(\pm E)$ as $t \to \pm\infty$. It follows that $C = \frac{m^2}{2E}\hat{\rho}(E)$. As $t \to -\infty$, we get contributions from both the reflection and the source. Hence $B = L - B_0$, where $L = \frac{m^2}{2E}\hat{\rho}(-E)$ and $B_0 = \frac{m^2}{2E}\hat{\rho}_0(-E)$ with ρ_0 the solution corresponding to $k = 0$. Thus, using the identity $T_L + R_L = 1$, we compute the transmission and reflection coefficients using only $\hat{\rho}_0(-E)$ and $\hat{\rho}(\pm E)$.

For a plot of R_L as a function of b, see Figure 5.12 (left panel). When b is small, Γ resembles a flat interface and thus R_L is close to 0. For larger values of b (say $b > 2$), the oscillations of the interface cause solutions to back-scatter, as R_L is approximately 1. The transition of R_L from 0 to 1 contains a small interval in b at which there is a sudden dip in R_L. See Figure 5.12 (center and right panels) for an illustration of the qualitatively different behavior of solutions corresponding to nearly identical interfaces. We suspect there may be other values of b (out of the range of values in Figure 5.12) for which sharp transitions in R_L occur, but postpone a thorough investigation of these critical values to future analyses.

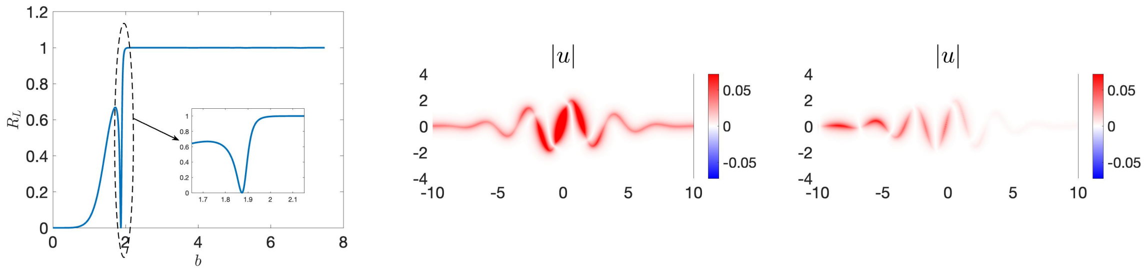

Figure 5.12: Scattering experiment for an interface parametrized by $\gamma(t) = 2e^{-0.05t^2}\sin(bt + 0.4)$, for $b \geq 0$. The source is located at $(-40, 1)$, and $(m, E) = (4, 1)$. The center and right panels illustrate the Green's function, u, corresponding to $b = 1.87$ and $b = 2.00$, respectively.

5.5 Proofs of main analytical results

This section is devoted to proving the statements from Section 5.2.1. First, we prove Theorems 5.2.1 and 5.2.4, verifying that u obtained by our boundary integral formulation solves the PDE (5.1.4, 5.1.5, 5.1.6, 5.1.7). We then prove Theorem 5.2.5 using Lemma 5.5.3 and Proposition 5.5.6, which in turn require Lemma 5.5.2 below. For completeness, we also state and prove Proposition 5.5.5–an extension of Lemma 5.5.3 which could be used interchangeably with Proposition 5.5.6 in our proof of Theorem 5.2.5. These propositions and lemmas provide bounds on $\|\mathcal{M}\|$ that guarantee bounded invertibility of $1 + \mathcal{M}$ in the $\lambda \to \infty$ limit. This section concludes with a proof of Theorem 5.2.7. The latter uses Lemma 5.5.7 below, which asserts that any solution of the homogeneous Klein-Gordon PDE (5.5.10) with complexified E must be trivial.

Let us begin with the proofs of Theorems 5.2.1 and 5.2.4.

Proof of Theorem 5.2.1. That (5.1.7) holds is a consequence of the exponential decay of $K_0(\omega|x - \gamma(t)|)$ in $|x - \gamma(t)|$ and the Lebesgue dominated convergence theorem. The latter also implies that (5.1.4) holds, while the jump conditions (5.1.5) follow immediately from the derivation of (5.2.16).

Let us now prove the outgoing condition (5.1.6). Since $f \in \mathcal{C}_c^\infty(\mathbb{R}^2)$, we have that

$u_i \in \mathcal{C}^\infty$ with u_i and all its derivatives decaying rapidly at infinity. Hence u_i satisfies (5.1.6), so it remains to consider u_s. We will treat each term on the right-hand side of $\mu = \rho + Q\rho$ separately. Set $r \neq 0$ and take $t_0 > 0$ sufficiently large so that $\{\gamma(t)+r\hat{n}(t) : t \geq t_0\} \cap \Gamma = \emptyset$. Note that our assumptions (5.1.1) and (5.1.2) on γ ensure that t_0 is well defined. Let $t \geq t_0$. Then $g(s) := \gamma(t)+r\hat{n}(t)-\gamma(s)$ is a smooth non-vanishing function satisfying $|g(s)| \gtrsim |t-s|$ for all $|t-s|$ sufficiently large. Thus for $j \in \{0,1\}$, $\partial_t^j K_0(\omega|\gamma(t)+r\hat{n}(t)-\gamma(s)|)$ is bounded and exponentially decaying in $|t-s|$. Since $\rho \in L^1$, this means

$$(\partial_t - iE)S_\omega[\rho](\gamma(t)+r\hat{n}(t)) = \frac{1}{2\pi}\int_{\mathbb{R}}(\partial_t - iE)K_0(\omega|\gamma(t)+r\hat{n}(t)-\gamma(s)|)\rho(s)\mathrm{d}s \qquad (5.5.1)$$

goes to 0 as $t \to \infty$. We now consider $Q\rho$. Again using that $\rho \in L^1$, it follows that

$$\begin{aligned}(\partial_t - iE)Q\rho(t) &= im^2\int_{-\infty}^{\infty}(\mathrm{sgn}(t-t')-1)e^{iE|t-t'|}\rho(t')\mathrm{d}t' \\ &= -2im^2\int_t^{\infty} e^{-iE(t-t')}\rho(t')\mathrm{d}t'\end{aligned} \qquad (5.5.2)$$

goes to 0 as $t \to \infty$. Writing

$$\partial_t S_\omega[Q\rho](\gamma(t)+r\hat{n}(t)) = \frac{1}{2\pi}\int_{\mathbb{R}}\partial_t K_0(\omega|\gamma(t)+r\hat{n}(t)-\gamma(s)|)Q\rho(s)\mathrm{d}s,$$

the strategy now is to show that $\partial_t K_0$ above is well approximated by $-\partial_s K_0$, so that we can then integrate by parts in s and apply (5.5.2). By the assumed exponential decay of γ'', it follows that

$$\Big|\partial_t|\gamma(t)+r\hat{n}(t)-\gamma(s)| + \partial_s|\gamma(t)+r\hat{n}(t)-\gamma(s)|\Big| \leq C_1 e^{-\tilde{\beta}\min\{t,s\}1_{\{s>0\}}} \qquad (5.5.3)$$

for some positive constants C_1 and $\tilde{\beta}$. Defining $R(t,s) := C_1\omega K_1(\omega|\gamma(t)+r\hat{n}(t)-\gamma(s)|)$, this means

$$\Big|(\partial_t + \partial_s)K_0(\omega|\gamma(t) + r\hat{n}(t) - \gamma(s)|)\Big| \le R(t,s)e^{-\tilde{\beta}\min\{t,s\}1_{\{s>0\}}},$$

and thus

$$\begin{aligned}\int_{\mathbb{R}} \Big|(\partial_t + \partial_s)K_0(\omega|\gamma(t) + r\hat{n}(t) - \gamma(s)|)Q\rho(s)\Big|\mathrm{d}s \\ \le \int_{-\infty}^{t/2} R(t,s)|Q\rho(s)|\mathrm{d}s + \int_{t/2}^{\infty} R(t,s)e^{-\tilde{\beta}\min\{t,s\}}|Q\rho(s)|\mathrm{d}s.\end{aligned}$$

Note that $\rho \in L^1$ implies $Q\rho \in L^\infty$. Since there exist positive constants C_2 and η such that $R(t,s) \le C_2 e^{-\eta|t-s|}$ for all $t \ge t_0$ and $s \in \mathbb{R}$, it follows that

$$\begin{aligned}\int_{-\infty}^{t/2} R(t,s)|Q\rho(s)|\mathrm{d}s + \int_{t/2}^{\infty} R(t,s)e^{-\tilde{\beta}\min\{t,s\}}|Q\rho(s)|\mathrm{d}s \\ \le \left(\frac{C_2}{\eta}e^{-\eta t/2} + \frac{2C_2}{\eta}e^{-\tilde{\beta}t/2}\right)\|Q\rho\|_\infty,\end{aligned}$$

hence

$$\lim_{t\to\infty} \int_{\mathbb{R}} \Big|(\partial_t + \partial_s)K_0(\omega|\gamma(t) + r\hat{n}(t) - \gamma(s)|)Q\rho(s)\Big|\mathrm{d}s = 0.$$

Integrating by parts, we obtain

$$\begin{aligned}&\Big|\int_{\mathbb{R}} (\partial_s + iE)K_0(\omega|\gamma(t) + r\hat{n}(t) - \gamma(s)|)Q\rho(s)\mathrm{d}s\Big| \\ &\quad = \Big|\int_{\mathbb{R}} K_0(\omega|\gamma(t) + r\hat{n}(t) - \gamma(s)|)((Q\rho)'(s) - iEQ\rho(s))\mathrm{d}s\Big| \\ &\quad \le \int_{-\infty}^{t/2} K_0(\omega|\gamma(t) + r\hat{n}(t) - \gamma(s)|)|(Q\rho)'(s) - iEQ\rho(s)|\mathrm{d}s \\ &\qquad + \big\|(Q\rho)' - iEQ\rho\big\|_{L^\infty[t/2,\infty)} \int_{t/2}^{\infty} K_0(\omega|\gamma(t) + r\hat{n}(t) - \gamma(s)|)\mathrm{d}s.\end{aligned}$$

The first term on the above right-hand side goes to 0 as $t \to \infty$ by the exponential decay of K_0. The second term goes to 0 by (5.5.2) and the fact that $\|K_0(\omega|\gamma(t) + r\hat{n}(t) - \gamma(\cdot)|)\|_{L^1} \leq C$ uniformly in $t \geq t_0$. We conclude that

$$\begin{aligned}|(\partial_t - iE)S_\omega[Q\rho](\gamma(t) + r\hat{n}(t))| \leq & \frac{1}{2\pi}\Big(\int_{\mathbb{R}} \Big|(\partial_t + \partial_s)K_0(\omega|\gamma(t) + r\hat{n}(t) - \gamma(s)|)Q\rho(s)\Big|\mathrm{d}s \\ & + \Big|\int_{\mathbb{R}}(\partial_s + iE)K_0(\omega|\gamma(t) + r\hat{n}(t) - \gamma(s)|)Q\rho(s)\mathrm{d}s\Big|\Big),\end{aligned}$$

with both terms on the right-hand side going to 0 as $t \to \infty$. We have thus shown that $\lim_{t\to\infty}(\partial_t - iE)u(\gamma(t) + s\hat{n}(t)) = 0$ The same argument applies when $t < 0$ (with ∂_t replaced by $-\partial_t$) and thus we have verified (5.1.6). □

Proof of Theorem 5.2.4. As before, (5.1.7) and (5.1.4) follow immediately from dominated Lebesgue, while the derivation of (5.2.23, 5.2.24) implies (5.1.5). We now prove (5.1.6). Recalling the definition of (μ, ρ) in (5.2.11), the same arguments from Theorem 5.2.1 imply that $\mu = \mu_0 + \mu_1$ and $\rho = \rho_0 + \rho_1$, where $\mu_0, \rho_0 \in L^1$, $\lim_{t\pm\infty}(\partial_t \mp iE)\mu_1(t) = 0$ and $\lim_{t\pm\infty}(\partial_t \mp iE)\rho_1(t) = 0$. Hence (following the proof of Theorem 5.2.1) $u_i + S_{\omega_j}[\mu]$ satisfies (5.1.6) for $j \in \{1, 2\}$. It remains to analyze $D_{\omega_j}[\rho]$. Fix $r > 0$, take $t_0 > 0$ sufficiently large so that $\{\gamma(t) + r\hat{n}(t) : t \geq t_0\} \cap \Gamma = \emptyset$, and let $t \geq t_0$. Defining $g(t, s) := \gamma(t) + r\hat{n}(t) - \gamma(s)$, we have

$$D_{\omega_2}[\rho](\gamma(t) + r\hat{n}(t)) = \frac{1}{2\pi}\int_{\mathbb{R}} \hat{n}(s) \cdot \frac{g(t, s)}{|g(t, s)|}K_1(\omega_2|g(t, s)|)\rho(s)\mathrm{d}s.$$

The exponential decay (5.1.1) of γ'' implies that

$$|(\partial_t + \partial_s)g(t, s)| + |(\partial_t + \partial_s)\hat{n}(s)| \leq Ce^{-\tilde{\beta}\min\{s,t\}1_{\{s>0\}}}$$

for some positive constants C and $\tilde{\beta}$. Since $K_1'(\omega_2|g(t, s)|)$ decays exponentially in $|t - s|$ with $\|K_1(\omega_2|g(t, \cdot)|)\|_{L_1} + \left\|K_1'(\omega_2|g(t, \cdot)|)\right\|_{L_1} \leq C$ uniformly in $t \geq t_0$, it follows (as in the proof of Theorem 5.2.1) that

$$\begin{aligned}
&|(\partial_t - iE)D_{\omega_2}[\rho_1](\gamma(t)+r\hat{n}(t))| \\
&\qquad \le \frac{1}{2\pi}\Big|\int_{\mathbb{R}}(\partial_t+\partial_s)\Big(\hat{n}(s)\cdot\frac{g(t,s)}{|g(t,s)|}K_1(\omega_2|g(t,s)|)\Big)\rho_1(s)\mathrm{d}s\Big| \\
&\qquad\quad + \frac{1}{2\pi}\Big|\int_{\mathbb{R}}\hat{n}(s)\cdot\frac{g(t,s)}{|g(t,s)|}K_1(\omega_2|g(t,s)|)(\partial_s - iE)\rho_1(s)\mathrm{d}s\Big|,
\end{aligned} \tag{5.5.4}$$

with both terms on the right-hand side going to 0 as $t\to\infty$. Similarly, the fact that $\rho_0 \in L^1$ directly implies that $(\partial_t - iE)D_{\omega_2}[\rho_0](\gamma(t)+r\hat{n}(t)) \to 0$ as $t\to\infty$. The limit $t\to-\infty$ is treated similarly, as is the case $r<0$. This completes the proof. □

Remark 5.5.1. *The solution u can actually satisfy a stronger outgoing condition than* (5.1.6). *It is possible to show that*

$$\lim_{t\to\pm\infty}\sup_{r\in[-1,1]}|(\pm\partial_t - iE)u(\gamma(t)+r\hat{n}(t))| = 0, \tag{5.5.5}$$

but this requires regularity of ρ (when $m_1 = m_2$) or σ (when $m_1 \neq m_2$). More specifically, the left-hand side of (5.5.3) *and $R(t,s) := C_1\omega K_1(\omega|\gamma(t)+r\hat{n}(t)-\gamma(s)|)$ can instead be bounded above by $C_1|t-s|e^{-\tilde{\beta}\min\{t,s\}1_{\{s>0\}}}$ and $\frac{C_2}{\sqrt{|t-s|^2+r^2}}e^{-\eta|t-s|}$, respectively, where the positive constants $C_1, C_2, \tilde{\beta}, \eta$ are independent of r. Thus all bounds after* (5.5.3) *can be shown to hold uniformly in r. The only obstruction to obtaining* (5.5.5) *is* (5.5.1)*, due to the singularity of $K_1 = -K_0'$ at zero. But if ρ were (weakly) differentiable with $\rho'(t)\to 0$ as $|t|\to\infty$, then $\mu := \mathcal{P}\rho$ would satisfy $\lim_{t\to\pm\infty}(\partial_t \mp iE)\mu(t) = 0$, meaning that all the bounds starting from* (5.5.3) *would hold with $Q\rho$ replaced by μ. Thus we would obtain* (5.5.5) *in this case. Similarly, if σ is weakly differentiable with $\sigma'(t)\to 0$ as $|t|\to\infty$, then* (5.5.5) *holds for the $m_1\neq m_2$ case.*

To guarantee this extra regularity of ρ and σ, we would need to show that $\mathcal{LP}$ and $\mathcal{L}_2\mathcal{P}_2$ are invertible on $H^1_\alpha := \{\rho\in L^2_\alpha : \rho'\in L^2_\alpha\}$. Such results are natural extensions of the ones *presented in Section 5.2.1 for L^2_α, and their proofs would likely use similar techniques to the ones presented below. However, we do not pursue this issue further here.*

The next part of this section is devoted to proving Theorem 5.2.5. As in the statement of the theorem, $m_0 > 0$ and $E_0 \in (-m_0, m_0) \setminus \{0\}$ will be fixed, with $\omega_0 := \sqrt{m_0^2 - E_0^2}$. The parameters m and E of our integral equation (5.2.3) will depend on the parameter $\lambda \in [1, \infty)$ via the relations $m = \lambda m_0$ and $E = \lambda E_0$. The constant α_* is defined above Theorem 5.2.5. Recall the definitions of $\mathcal{L}, \mathcal{P}, \mathcal{L}_0$ and $\mathcal{M}$ in (5.2.2), (5.2.12) and (5.2.13). We will use $\|\cdot\|$ to denote the operator norm. More specifically, if $\mathcal{B}_1$ and $\mathcal{B}_2$ are Banach spaces and $\mathcal{A} : \mathcal{B}_1 \to \mathcal{B}_2$ is a linear operator, then $\|\mathcal{A}\| := \sup\{\|\mathcal{A}\psi\|_2 : \|\psi\|_1 = 1\}$, where $\|\cdot\|_j$ denotes the norm on $\mathcal{B}_j$.

We begin with the following important lemmas.

Lemma 5.5.2. *For all $\alpha \in (0, \alpha_*]$, the operator $(\mathcal{L}_0\mathcal{P})^{-1}$ is bounded on L^2_α with $\left\|(\mathcal{L}_0\mathcal{P})^{-1}\right\| \leq C$ uniformly in $\lambda \in [1, \infty)$.*

Proof. Fix $\alpha \in (0, \alpha_*]$. By (5.2.20) we know that $(\mathcal{L}_0\mathcal{P})^{-1} = (1 + R_0)(1 + R_1)$, where R_0 and R_1 are convolutions by $r_0 := mK_0(\omega|\cdot|)$ and $r_1 := \frac{(i-2)m^2}{2\zeta} e^{i\zeta|\cdot|}$, respectively, with $\zeta := a_+ + ia_-$ and

$$a_\pm := \sqrt{\frac{\sqrt{4m_0^4 + E_0^4} \pm E_0^2}{2}}.$$

Thus there exists $r \in L^1$ such that $e^{\alpha|\cdot|}r(\cdot) \in L^1$ and $|r_j(t)| \leq \lambda r(\lambda(t))$ for all $\lambda \in [1, \infty)$ and $j \in \{1, 2\}$. Using the identity $\|g_1 * g_2\|_{L^2} \leq \|g_1\|_{L^1} \|g_2\|_{L^2}$ with $g_1(t) = \lambda e^{\alpha|t|} r(\lambda|t|)$ and $g_2(t) = e^{\alpha|t|}|\rho|(t)$, we obtain that for $\rho \in L^2_\alpha$ and $j \in \{1, 2\}$,

$$\begin{aligned}
\|R_j\rho\|^2_{L^2_\alpha} &\leq \int_{\mathbb{R}} e^{2\alpha|t|} \Big(\int_{\mathbb{R}} \lambda r(\lambda|t - t'|)\rho(t')\mathrm{d}t' \Big)^2 \mathrm{d}t \\
&\leq \int_{\mathbb{R}} \Big(\int_{\mathbb{R}} \lambda e^{\alpha|t-t'|} r(\lambda|t - t'|) e^{\alpha|t'|}|\rho|(t')\mathrm{d}t' \Big)^2 \mathrm{d}t
\end{aligned}$$

is bounded uniformly in $\lambda \in [1, \infty)$. This completes the proof. $\square$

Lemma 5.5.3. *For all $\alpha \in (0, \alpha_*]$ and $\lambda \in [1, \infty)$, the operator $\mathcal{M}$ is Hilbert-Schmidt (hence compact) on L^2_α.*

Proof. Fix $\alpha \in (0, \alpha_*]$ and $\lambda \in [1, \infty)$, and note that $L^2_\alpha \subset L^1 \cap L^2$. Define $A_1 : L^2 \to L^2_\alpha, A_2 : L^2 \to L^2, A_3 : L^2_\alpha \to L^2$ by

$$A_1 = W_\alpha^{-1}, \qquad A_2 = W_\alpha(\mathcal{L}_0 - \mathcal{L})W_\alpha, \qquad A_3 = W_\alpha^{-1}\mathcal{P},$$

where W_α is point-wise multiplication by w_α. Our strategy is to bound each term on the right-hand side of $\mathcal{M} = (\mathcal{L}_0\mathcal{P})^{-1}A_1A_2A_3$. We immediately have $\|A_1\rho\|_{L^2_\alpha} = \|\rho\|_{L^2}$, so A_1 is bounded. Using that

$$|\mathcal{P}\rho|(t) \leq |\rho|(t) + \frac{m^2}{|E|}\|\rho\|_{L^1} \leq |\rho|(t) + C\|\rho\|_{L^2_\alpha}, \tag{5.5.6}$$

we have $\|A_3\rho\|_{L^2} \leq C\|\rho\|_{L^2_\alpha}$, hence A_3 is also bounded. By Lemma 5.5.2, $(\mathcal{L}_0\mathcal{P})^{-1}$ is bounded on L^2_α.

It remains to show that A_2 is Hilbert-Schmidt. To do so, we will prove exponential decay of the kernel of $\mathcal{L}_0-\mathcal{L}$ using the decay properties of K_0 and the fact that our interface rapidly converges to a straight line at infinity (5.1.1). Let $\ell_\Delta(t,s) = K_0(\omega|\gamma(t)-\gamma(s)|) - K_0(\omega|t-s|)$ so that $-\frac{m}{\pi}\ell_\Delta(t,s)$ is the kernel of $\mathcal{L} - \mathcal{L}_0$. Since K_0 and $K_1 = -K_0'$ are both positive and monotonically decreasing, and $|\gamma(t) - \gamma(s)| \leq |t-s|$, it follows that

$$0 \leq \ell_\Delta(t,s) = \int_{\omega|\gamma(t)-\gamma(s)|}^{\omega|t-s|} K_1(z)\mathrm{d}z \leq \omega(|t-s| - |\gamma(t)-\gamma(s)|)K_1(\omega|\gamma(t)-\gamma(s)|).$$

Hence

$$0 \leq \ell_\Delta(t,s) \leq \omega(|t-s| - |\gamma(t)-\gamma(s)|)K_1(c\omega|t-s|), \tag{5.5.7}$$

where $c > 0$ is defined by (5.1.3). The factor $K_1(c\omega|t-s|)$ decays exponentially in $|t-s|$ but has a singularity at $t = s$. To show that ℓ_Δ is bounded and decays exponentially in $|t| + |s|$, we will control the difference $|t - s| - |\gamma(t) - \gamma(s)|$.

By smoothness of γ, for every $s, t \in \mathbb{R}$ there exist $r_1, r_2 \in [\min\{s,t\}, \max\{s,t\}]$ such that

$$\gamma(t) = \gamma(s) + (t-s)\gamma'(s) + \frac{1}{2}(t-s)^2\gamma''(s) + \frac{1}{3!}(t-s)^3(\gamma_1'''(r_1), \gamma_2'''(r_2)). \tag{5.5.8}$$

Since $|\gamma'| \equiv 1$ and thus $\gamma' \cdot \gamma'' \equiv 0$, we have

$$\gamma'(s) \cdot (\gamma(t) - \gamma(s)) = t - s + \frac{1}{3!}(t-s)^3\gamma'(s) \cdot (\gamma_1'''(r_1), \gamma_2'''(r_2)).$$

Multiplying both sides by $t - s$ and using (5.5.8) to expand $(t-s)\gamma'(s)$, it follows that

$$\begin{aligned}|\gamma(t) - \gamma(s)|^2 = (t-s)^2 + \frac{1}{3!}(t-s)^4\gamma'(s) \cdot (\gamma_1'''(r_1), \gamma_2'''(r_2)) + \frac{1}{2}(t-s)^2\gamma''(s)(\gamma(t) - \gamma(s)) \\ + \frac{1}{3!}(t-s)^3(\gamma_1'''(r_1), \gamma_2'''(r_2)) \cdot (\gamma(t) - \gamma(s)).\end{aligned}$$

Again using (5.5.8) to expand $\gamma(t) - \gamma(s)$ on the bottom line, we obtain that

$$|\gamma(t) - \gamma(s)|^2 \leq (t-s)^2 + CJ(s,t)(t-s)^4, \qquad J(s,t) := |\gamma''|_{s,t}^2 + |\gamma'''|_{s,t}$$

for some $C > 0$, where the semi-norm $|\cdot|_{s,t}$ is defined by

$$|\eta|_{s,t} := \|\eta\|_{L^\infty[\min\{s,t\},\max\{s,t\}]}.$$

This implies $0 \leq |t-s| - |\gamma(t) - \gamma(s)| \leq CJ(s,t)|t-s|^3$. From the rapid decay (5.1.1) of

$|\gamma''|^2 + |\gamma'''|$ at infinity, it follows that

$$0 \leq |t-s| - |\gamma(t) - \gamma(s)| \leq \frac{C_0}{\sqrt{2}}|t-s|^3 e^{-\beta\chi(s,t)}, \qquad \chi(s,t) := \begin{cases} \min\{|s|,|t|\}, & st > 0 \\ 0, & \text{else.} \end{cases}$$

Using (5.5.7), we have

$$0 \leq \ell_\Delta(t,s) \leq \frac{\omega}{\sqrt{2}} C_0 |t-s|^3 e^{-\beta\chi(s,t)} K_1(c\omega|t-s|). \tag{5.5.9}$$

By definition of α_*, we conclude that

$$\int_{\mathbb{R}^2} w_\alpha^2(t) w_\alpha^2(s) \ell_\Delta^2(t,s) \mathrm{d}t\mathrm{d}s < \infty.$$

This means A_2 is Hilbert-Schmidt and the proof is complete. $\square$

Henceforth, $\|\cdot\|_2$ denotes the Hilbert-Schmidt norm.

Remark 5.5.4. *Since the constant C in* (5.5.6) *is proportional to* $1/|E|$, *we have shown that* $\|\mathcal{M}\|_2 \leq C/|E|$ *as* $E \to 0$. *The singularity at* $E = 0$ *should not be surprising, as outgoing and incoming conditions at infinity are the same in this case. It turns out that an appropriate linear combination of outgoing and incoming conditions produces an operator that behaves better in the* $E \to 0$ *limit. Indeed, we could have instead defined* $Q : L^2_\alpha \to L^\infty$ *by* $Q\rho(t) = \frac{i}{2E}\int_{-\infty}^{\infty}(e^{iE|t-t'|} - e^{-iE|t-t'|})\rho(t')\mathrm{d}t'$, *which is bounded uniformly in* E *(for any* $\alpha > 0$*). The resulting solution would now look like* $\sin(E|t|)$ *as* $|t| \to \infty$.

Lemma 5.5.3 implies that if (5.2.13) does not have a unique solution ρ, then the kernel of $1 + \mathcal{M}$ is a nontrivial finite-dimensional subspace of L^2_α. An extension of Lemma 5.5.3 is the following

Proposition 5.5.5. *For any* $\alpha \in (0, \alpha_*]$, $\|\mathcal{M}\|_2 \leq C/\sqrt{\lambda}$ *as* $\lambda \to \infty$.

Proof. Suppose $\lambda \geq 1$. As in the proof of Lemma 5.5.3, we will bound each factor on the right-hand side of $\mathcal{M} = (\mathcal{L}_0\mathcal{P})^{-1}A_1A_2A_3$. By Lemma 5.5.2, the operator norm of $(\mathcal{L}_0\mathcal{P})^{-1}$ on L^2_α is bounded uniformly in λ. From (5.5.6) it is clear that $\|A_3\| \leq C\lambda$. Since A_1 is independent of λ, it remains to bound $\|A_2\|_2$.

The kernel of A_2 is $k(t,s) = \frac{m}{\pi}w_\alpha(t)\ell_\Delta(t,s)w_\alpha(s)$, with $\ell_\Delta(t,s) = K_0(\omega|\gamma(t)-\gamma(s)|) - K_0(\omega|t-s|)$ as before. From (5.5.9) it follows that

$$k^2(t,s) \leq \Big(\frac{m\omega C_0}{\sqrt{2\pi}}\Big)^2 w_\alpha^2(t)w_\alpha^2(s)(t-s)^6 e^{-2\beta\chi(s,t)}K_1^2(c\omega|t-s|).$$

Performing the change of variables $(\xi,\zeta) := (t-s, t+s)$ and using the fact that $|\zeta+\xi|+|\zeta-\xi| \leq |\zeta+\lambda\xi|+|\zeta-\lambda\xi|$ and $\chi(\frac{\zeta-\lambda\xi}{2},\frac{\zeta+\lambda\xi}{2}) \leq \chi(\frac{\zeta-\xi}{2},\frac{\zeta+\xi}{2})$ for all $\lambda \geq 1$ and $\xi,\zeta \in \mathbb{R}$, it follows that

$$\begin{aligned}\|k\|_{L^2}^2 &\leq \frac{1}{2}\Big(\frac{m\omega C_0}{\sqrt{2\pi}}\Big)^2 \int_{\mathbb{R}^2} w_\alpha^2\Big(\frac{\zeta+\lambda\xi}{2}\Big)w_\alpha^2\Big(\frac{\zeta-\lambda\xi}{2}\Big)\xi^6 e^{-2\beta\chi(\frac{\zeta-\lambda\xi}{2},\frac{\zeta+\lambda\xi}{2})}K_1^2(c\omega_0\lambda|\xi|)\mathrm{d}\zeta\mathrm{d}\xi \\ &= \frac{1}{2\lambda^7}\Big(\frac{m\omega C_0}{\sqrt{2\pi}}\Big)^2 \int_{\mathbb{R}^2} w_\alpha^2\Big(\frac{\zeta+\xi}{2}\Big)w_\alpha^2\Big(\frac{\zeta-\xi}{2}\Big)\xi^6 e^{-2\beta\chi(\frac{\zeta-\xi}{2},\frac{\zeta+\xi}{2})}K_1^2(c\omega_0|\xi|)\mathrm{d}\zeta\mathrm{d}\xi.\end{aligned}$$

Since the above integral is finite (by definition of α_*) and independent of λ, we have shown that $\|k\|_{L^2} \leq C/\lambda^{3/2}$ for all λ sufficiently large. Thus

$$\|\mathcal{M}\|_2 \leq \left\|(\mathcal{L}_0\mathcal{P})^{-1}\right\| \|A_1\| \|A_2\|_2 \|A_3\| \leq C/\sqrt{\lambda}$$

and the proof is complete. □

The above result implies that $\|\mathcal{M}\| \to 0$ as $\lambda \to \infty$. However, it is possible to get faster decay of $\|\mathcal{M}\|$ in λ.

Proposition 5.5.6. *For any $\alpha \in (0,\alpha_*]$, $\|\mathcal{M}\| \leq C/\lambda$ as $\lambda \to \infty$.*

Proof. Recall Lemma 5.5.2, which states that $\left\|(\mathcal{L}_0\mathcal{P})^{-1}\right\| \leq C$ uniformly in λ. Thus it remains to bound the norm of $(\mathcal{L}-\mathcal{L}_0)\mathcal{P}$. We will bound the terms $\mathcal{L}-\mathcal{L}_0$ and $(\mathcal{L}-\mathcal{L}_0)Q$ separately.

We begin with the latter. We have that $\|Q\rho\|_\infty \leq \frac{Cm^2}{E}\|\rho\|_{L^2_\alpha}$, thus for $(\mathcal{L}-\mathcal{L}_0)Q$ it suffices to bound $\mathcal{L}-\mathcal{L}_0$ from L^∞ to L^2_α. The kernel of $\mathcal{L}-\mathcal{L}_0$ is $-\frac{m}{\pi}\ell_\Delta(t,s)$, where $\ell_\Delta(t,s) = K_0(\omega|\gamma(t)-\gamma(s)|) - K_0(\omega|t-s|)$. Using (5.5.9), it follows that for $\rho \in L^\infty$ we have

$$
\begin{aligned}
|(\mathcal{L}-\mathcal{L}_0)\rho|(t) &\leq \frac{m}{\pi}\|\rho\| \int_{\mathbb{R}} \ell_\Delta(t,s)\mathrm{d}s \\
&\leq C\|\rho\|\lambda^2 \int_{\mathbb{R}} |t-s|^3 e^{-\beta\chi(s,t)} K_1(c\omega|t-s|)\mathrm{d}s \\
&=: C\|\rho\|\lambda^2 I,
\end{aligned}
$$

where $\|\rho\| := \|\rho\|_\infty$. For concreteness, suppose $t \geq 0$. This means

$$
\chi(s,t) = \begin{cases} 0, & s < 0 \\ s, & 0 \leq s \leq t \\ t, & s > t \end{cases}
$$

so that

$$
I = \int_{-\infty}^0 \kappa_\omega(t-s)\mathrm{d}s + \int_0^t \kappa_\omega(t-s)e^{-\beta s}\mathrm{d}s + \int_t^\infty \kappa_\omega(t-s)e^{-\beta t}\mathrm{d}s =: I_1 + I_2 + I_3,
$$

where we have defined $\kappa_\omega(x) := |x|^3 K_1(c\omega|x|)$. Recall that by definition of α_*, we have

$0 < \alpha_* < \beta$ and $\kappa_1(x) \le Ce^{-\alpha_*|x|}$ for all $x \in \mathbb{R}$. Thus

$$\begin{aligned}
I_1 &\le C\omega^{-4} \int_t^\infty e^{-\alpha_* s} \mathrm{d}s = \frac{C}{\alpha_* \omega^4} e^{-\alpha_* t} = C_1 \omega^{-4} e^{-\alpha_* t}, \\
I_2 &= \int_0^t \kappa_\omega(s) e^{-\beta(t-s)} \mathrm{d}s \le C\omega^{-4} \int_0^t e^{-\alpha_* s} e^{-\beta(t-s)} \mathrm{d}s \\
&\le \frac{C}{(\beta - \alpha_*)\omega^4} e^{-\beta t}(e^{(\beta-\alpha_*)t} - 1) \le C_2 \omega^{-4} e^{-\alpha_* t}, \\
I_3 &= e^{-\beta t} \int_{-\infty}^0 \kappa_\omega(s) \mathrm{d}s \le \frac{C}{\alpha_* \omega^4} e^{-\beta t} = C_3 \omega^{-4} e^{-\beta t} \le C_3 \omega^{-4} e^{-\alpha_* t}
\end{aligned}$$

uniformly in $t \ge 0$, for some positive constants C_1, C_2 and C_3. Repeating the same argument for $t < 0$ and recalling that $\alpha < \alpha_*$, it follows that $\|(\mathcal{L} - \mathcal{L}_0)\rho\|_{L^2_\alpha} \le \frac{C\|\rho\|}{\lambda^2}$. Thus we have shown that $\|(\mathcal{L} - \mathcal{L}_0)Q\| \le C/\lambda$.

It remains to bound $\mathcal{L} - \mathcal{L}_0$ from L^2_α to itself. We already showed in the proof of Proposition 5.5.5 that $A_2 = W_\alpha(\mathcal{L}_0 - \mathcal{L})W_\alpha$ is Hilbert-Schmidt on L^2 with $\|A_2\|_2 \le C/\lambda^{3/2}$. This means $\|\mathcal{L} - \mathcal{L}_0\|_{L^2_\alpha \to L^2_\alpha} \le C/\lambda^{3/2}$ and the proof is complete. □

Finally, we prove the first well-posedness result of Section 5.2.1.

Proof of Theorem 5.2.5. Fix $\alpha \in (0, \alpha_*]$ and $\delta \in (0, \alpha)$.

Since $\mathcal{M} : L^2_\alpha \to L^2_\alpha$ is holomorphic in $\lambda \in [1, \infty) \times (-\delta, \delta)$, we apply Lemma 5.5.3, Proposition 5.5.6 and Kato perturbation theory [58, Theorem VII.1.9] to prove that $\mathcal{M}$ has an eigenvalue of -1 for only a finite number of $\lambda \in [1, \infty)$. The result then follows from (5.2.13). □

As opposed to the above, Theorem 5.2.7 does not require $\mathcal{M}$ to be small in any limit. Instead, we show that -1 belongs to the resolvent set of $\mathcal{M}$ whenever $\Im E > 0$. To this end, we state the following

Lemma 5.5.7. *Fix $m > 0$. For all $E \in \mathbb{C}$ with $0 < |\Re E| < m$ and $\Im E \ne 0$, if $u \in H^1(\mathbb{R}^2)$ solves* (5.5.10) *below, then $u \equiv 0$.*

Proof. Integrating by parts, we see that

$$\int_{\Omega_j} |\nabla u|^2 \mathrm{d}x = -\omega^2 \int_{\Omega_j} |u|^2 \mathrm{d}x + \varepsilon_j \int_\Gamma u\hat{n} \cdot \nabla u \mathrm{d}t,$$

where $\varepsilon_1 = 1$ and $\varepsilon_2 = -1$. Taking the sum over j and using the second line of (5.5.10), we obtain

$$\int_{\mathbb{R}^2} |\nabla u|^2 \mathrm{d}x + \omega^2 \int_{\mathbb{R}^2} |u|^2 \mathrm{d}x = 2m \int_\Gamma |u|^2 \mathrm{d}t$$

Taking the imaginary part of both sides, we conclude that $\int_{\mathbb{R}^2} |u|^2 \mathrm{d}x = 0$ and the result is complete. $\square$

Using the above lemma, we now prove the second well-posedness result from Section 5.2.1.

Proof of Theorem 5.2.7. Fix $\varepsilon > 0$ and for $\alpha > 0$ define $Z_{\alpha,\varepsilon} := ([-m+\varepsilon, -\varepsilon] \cup [\varepsilon, m-\varepsilon]) \times (-\alpha/2, \alpha/2) \subset \mathbb{C}$. The same arguments as above show that $\mathcal{M} : L^2_\alpha \to L^2_\alpha$ is Hilbert-Schmidt and holomorphic in $E \in Z_{\alpha,\varepsilon}$ for all $\alpha > 0$ sufficiently small.

Fix $E \in Z_{\alpha,\varepsilon}$ such that $\Im E > 0$. By contradiction suppose $\mathcal{M}$ has an eigenvalue of -1. Then there exists $0 \neq \rho \in L^2_\alpha$ such that $(1 + \mathcal{M})\rho = 0$. Letting $\mu := \mathcal{P}\rho$, it follows that $u = S_\omega[\mu]$ solves the homogeneous problem

$$\begin{cases} \Delta u(x) - \omega^2 u(x) = 0, \quad x \in \mathbb{R}^2 \setminus \Gamma, \\ [[\hat{n} \cdot \nabla u]](\gamma(t)) = -2mu(\gamma(t)), \quad t \in \mathbb{R}, \\ [[u]](\gamma(t)) = 0, \quad t \in \mathbb{R}, \end{cases} \tag{5.5.10}$$

where $\omega^2 = m^2 - E^2$. Since E has positive imaginary part, Q is bounded from L^2_α to itself, meaning that $\mu \in L^2_\alpha$. It follows that u and ∇u decay rapidly at infinity; for example, $u \in H^1(\mathbb{R}^2)$. Lemma 5.5.7 then implies that $S_\omega[\mu] \equiv 0$; hence $\mu \equiv 0$ by (5.1.12). It follows from (5.2.18) that $0 = \tilde{\mu}(\xi) = (1 - \frac{2im^2}{\xi^2 - E^2})\tilde{\rho}(\xi)$, from which we conclude that $\rho \equiv 0$, a contradiction. Indeed, if α is chosen sufficiently small, then 1 is not in the image of the map $\mathbb{R} \ni \xi \mapsto \frac{2im^2}{\xi^2 - E^2}$. We have thus shown that -1 is not an eigenvalue of $\mathcal{M}$ whenever $E \in Z_{\alpha,\varepsilon}$ has positive imaginary part. This means we can again apply [58, Theorem VII.1.9] to complete the result. $\square$

Remark 5.5.8. *It is crucial that $Z_{\alpha,\varepsilon}$ be bounded away from* 0 *as Q is not holomorphic there. Thus we cannot guarantee that the number of "bad" E-values near* 0 *is finite. As suggested by Remark 5.5.4, one could redefine Q by $Q\rho(t) = \frac{i}{2E}\int_{-\infty}^{\infty}(e^{iE|t-t'|} - e^{-iE|t-t'|})\rho(t')\mathrm{d}t'$ to make it holomorphic, but then the outgoing conditions* (5.1.6) *would not be satisfied.*

APPENDIX A

PSEUDO-DIFFERENTIAL CALCULUS

A.1 Notation and functional setting

Given a bounded linear operator $A : \mathcal{H} \to \mathcal{H}$ for $\mathcal{H}$ a Hilbert space, we denote by A^* its adjoint and $\|A\|$ its operator norm. If, in addition, A^*A is compact, then by the spectral theorem, A^*A admits a countable collection of eigenvalues $\{\lambda_j\} \subset [0,\infty)$ converging to 0. The operator A is Hilbert-Schmidt if $\|A\|_2 := \sum_j \lambda_j < \infty$ and trace-class if $\|A\|_1 := \sum_j \sqrt{\lambda_j} < \infty$. If A is trace-class, we define the trace of A by

$$\operatorname{Tr} A := \sum_{j\in\mathbb{N}} (\psi_j, A\psi_j),$$

where $\{\psi_j\}_{j\in\mathbb{N}}$ is any Hilbert basis of $\mathcal{H}$ (the trace is independent of the chosen Hilbert basis).

Weyl Quantization. See [34, Chapter 7]. Let $\mathcal{S}(\mathbb{R}^d)\otimes\mathbb{C}^n$ be the Schwartz space of vector-valued functions and $\mathcal{S}'(\mathbb{R}^d)\otimes\mathbb{C}^n$ its dual. Given a parameter $h \in (0,1]$ and a symbol $a(x,\xi;h) = a \in \mathcal{S}'(\mathbb{R}^d\times\mathbb{R}^d)\otimes\mathbb{C}^{n\times n}$, we define the Weyl quantization of a as the operator

$$\operatorname{Op}_h(a)\psi(x) := \frac{1}{(2\pi h)^d}\int_{\mathbb{R}^{2d}} e^{i(x-y)\cdot\xi/h} a(\frac{x+y}{2},\xi;h)\psi(y)dyd\xi, \qquad \psi\in\mathcal{S}(\mathbb{R}^d)\otimes\mathbb{C}^n. \tag{A.1.1}$$

When a is polynomial in ξ, it follows that $\operatorname{Op}_h(a)$ is a differential operator. We denote by $\operatorname{Op} a = \operatorname{Op}_1 a$ for $h = 1$.

Any bounded matrix-valued operator A from $\mathcal{S}(\mathbb{R}^d)\otimes\mathbb{C}^n$ to $\mathcal{S}'(\mathbb{R}^d)\otimes\mathbb{C}^n$ admits a

Schwartz kernel $k_A \in \mathcal{S}'(\mathbb{R}^d \times \mathbb{R}^d) \otimes \mathbb{C}^{n\times n}$ such that

$$A\psi(x) = \int_{\mathbb{R}^d} k_A(x,y)\psi(y)dy, \qquad \psi \in \mathcal{S}(\mathbb{R}^d) \otimes \mathbb{C}^n.$$

If $A = \operatorname{Op}(a)$, then

$$a(x,\xi) = \int_{\mathbb{R}^d} e^{-iy\cdot\xi} k_A(x + \frac{y}{2}, x - \frac{y}{2})dy.$$

Order functions and symbol classes. See [20] and [34, Chapter 7]. For $(x,\xi) = X \in \mathbb{R}^{2d}$, we define $\langle X \rangle := \sqrt{1+|X|^2}$. A function $\mathfrak{m} : \mathbb{R}^{2d} \to [0,\infty)$ is called an order function if there exist constants $C_0 > 0$, $N_0 > 0$ such that $\mathfrak{m}(X) \le C_0 \langle X - Y\rangle^{N_0}\mathfrak{m}(Y)$ for all $X, Y \in \mathbb{R}^{2d}$. Note that $\langle X\rangle^p$ and $\langle X_\pm \rangle$ are order functions for all $p \in \mathbb{R}$, where $X_+ := \max\{X, 0\}$ (with the max defined element-wise) and $X_- := -(-X)_+$. Moreover, if $\mathfrak{m}_1$ and $\mathfrak{m}_2$ are order functions, then so is $\mathfrak{m}_1\mathfrak{m}_2$.

We say that $a \in S(\mathfrak{m})$ if for every $\alpha \in \mathbb{N}^{2d}$, there exists $C_\alpha > 0$ such that $|\partial^\alpha a(X;h)| \le C_\alpha \mathfrak{m}(X)$ for all $X \in \mathbb{R}^{2d}$ and $h \in (0,1]$. We write $S(\mathfrak{m}^{-\infty})$ to denote the intersection over $s \in \mathbb{N}$ of $S(\mathfrak{m}^{-s})$. For $\delta \in [0,1]$ and $k \in \mathbb{R}$, we say that $a(X;h) \in S^k_\delta(\mathfrak{m})$ if for every $\alpha \in \mathbb{N}^{2d}$, there exists $C_\alpha > 0$ such that

$$|\partial^\alpha a(X;h)| \le C_\alpha \mathfrak{m}(X) h^{-\delta|\alpha|-k}, \tag{A.1.2}$$

uniformly in $X \in \mathbb{R}^{2d}$ and $h \in (0,1]$. If either k or δ are omitted, they are assumed to be zero. We will always write the order function $\mathfrak{m}$ when using these symbol classes.

By [34, Chapter 7], we know that if $a \in S(\mathfrak{m}_1)$ and $b \in S(\mathfrak{m}_2)$, then $\operatorname{Op}_h(c) := \operatorname{Op}_h(a)\operatorname{Op}_h(b)$ is a pseudo-differential operator, with

$$c(x,\xi;h) = (a\sharp_h b)(x,\xi;h) := \Big(e^{i\frac{h}{2}(\partial_x\cdot\partial_\zeta - \partial_y\cdot\partial_\xi)} a(x,\xi;h)b(y,\zeta;h)\Big)\Big|_{y=x,\zeta=\xi}$$

and $c \in S(\mathfrak{m}_1\mathfrak{m}_2)$. See also Proposition A.2.1 for explicit bounds on c.

For $m \in \mathbb{Z}$, define the standard Hilbert spaces

$$\mathcal{H}^m := \{\Psi \in \mathcal{S}'(\mathbb{R}^2) \otimes \mathbb{C}^n \quad | \quad \partial_\alpha \Psi \in \mathcal{H} \quad \forall\, |\alpha| \leq m\}. \tag{A.1.3}$$

Following [20, 55, 61], we define the Hörmander class $S^m_{1,0}$ to be the space of symbols $a(x,\xi)$ that satisfy

$$|(\partial^\alpha_\xi \partial^\beta_x a)(x,\xi)| \leq C_{\alpha,\beta} \langle \xi \rangle^{m-|\alpha|}; \qquad \alpha, \beta \in \mathbb{N}^d. \tag{A.1.4}$$

We define $ES^m_{1,0}$ to be the space of *Hermitian-valued* symbols $a(x,\xi)$ that satisfy (A.1.4) and $|a_{\min}(x,\xi)| \geq c\langle \xi \rangle^m - 1$ for some $c > 0$, where $a_{\min}$ is the smallest-magnitude eigenvalue of a.

If $\mathcal{A}$ is a symbol class (e.g. $S(\mathfrak{m}), S^m_{1,0}, ES^m_{1,0}$), we write $A \in \mathrm{Op}(\mathcal{A})$ to mean that $A = \mathrm{Op}(a)$ for some $a \in \mathcal{A}$. In the case $\mathcal{A} = S(\mathfrak{m})$, the notation $A \in \mathrm{Op}_h(S(\mathfrak{m}))$ means that $A = \mathrm{Op}_h(a)$ for some $a \in S(\mathfrak{m})$.

Helffer-Sjöstrand formula. See [34, Chapter 8]. Given $f \in \mathcal{C}^\infty_c(\mathbb{R})$, there exists an almost analytic extension $\tilde{f} \in \mathcal{C}^\infty_c(\mathbb{C})$ that satisfies

$$|\bar{\partial} \tilde{f}| \leq C_N |\omega|^N, \quad N \in \{0, 1, 2, \dots\}; \qquad \tilde{f}(\lambda) = f(\lambda), \quad \lambda \in \mathbb{R}. \tag{A.1.5}$$

Here, $z =: \lambda + i\omega$ and $\bar{\partial} := \frac{1}{2}\partial_\lambda + \frac{i}{2}\partial_\omega$. We now recall [34, Theorem 8.1]. If H is a self-adjoint operator on a Hilbert space, then

$$f(H) = -\frac{1}{\pi} \int \bar{\partial} \tilde{f}(z)(z - H)^{-1} d^2 z, \tag{A.1.6}$$

where $d^2 z$ is the Lebesgue measure on $\mathbb{C}$. (A.1.6) is known as the Helffer-Sjöstrand formula, and we use it repeatedly in this thesis.

Trace-class operators. See [34, Chapter 9]. Suppose $\mathfrak{m} \in L^1(\mathbb{R}^{2d})$, and $|\partial^\alpha a(x,\xi;h)| \leq C_\alpha \mathfrak{m}(x,\xi)$ for all $\alpha \in \mathbb{N}^{2d}$ and $h \in (0,1]$ (meaning that $a \in S(\mathfrak{m})$). Then $\mathrm{Op}_h(a)$ is trace-class with $\|\mathrm{Op}_h(a)\|_1 \leq C \max_{|\alpha|\leq 2d+1} C_\alpha \|\mathfrak{m}\|_{L^1}$ and

$$\mathrm{Tr}\,\mathrm{Op}_h(a) = \frac{1}{(2\pi h)^d} \int_{\mathbb{R}^{2d}} \mathrm{tr}\, a(x,\xi;h) dx d\xi, \tag{A.1.7}$$

where C depends only on d and tr is the standard matrix trace. To obtain the above equality, we use [34, Theorem 9.4] to write

$$\begin{aligned} \mathrm{Tr}\,\mathrm{Op}_h(a(x,\xi;h)) &= \mathrm{Tr}\,\mathrm{Op}_1(a(x,h\xi;h)) \\ &= \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} \mathrm{tr}\, a(x,h\xi;h) dx d\xi = \frac{1}{(2\pi h)^d} \int_{\mathbb{R}^{2d}} \mathrm{tr}\, a(x,\xi;h) dx d\xi. \end{aligned}$$

The results from [20, 34] that were used in this section are stated for scalar symbols. They extend to the matrix-valued case; see [19].

A.2 Composition calculus

For $\mathfrak{m} : \mathbb{R}^{2d} \to [0,\infty)$ an order function, $u \in S(\mathfrak{m})$ and $N \in \mathbb{N}$, define

$$\tilde{C}_N(u,\mathfrak{m}) := \sum_{|\alpha|\leq N} \inf\{C > 0 : |\partial^\alpha u| \leq C\mathfrak{m}\}.$$

For $u_1, u_2 \in \mathcal{C}^\infty(\mathbb{R}^{2d}; \mathbb{C}^{n\times n})$ and $N \in \mathbb{N}$, define

$$\begin{aligned} T_N(u_1,u_2) &= (T_N(u_1,u_2))(x,\xi) \\ &:= \sum_{j=0}^{N-1} \Big(\frac{(ih(D_\xi \cdot D_y - D_x \cdot D_\eta)/2)^j}{j!} u_1(x,\xi) u_2(y,\eta) \Big)|_{y=x,\eta=\xi}. \end{aligned}$$

Proposition A.2.1. *Let $\mathfrak{m}_1, \mathfrak{m}_2 : \mathbb{R}^{2d} \to [0,\infty)$ be order functions. Then there exists $s \in \mathbb{N}$*

such that for every $N \in \mathbb{N}$ *and* $\alpha \in \mathbb{N}^{2d}$*,*

$$|\partial^\alpha(u_1 \sharp_h u_2 - T_N)| \leq C_{\alpha,N} \sum_{j=0}^{|\alpha|} \tilde{C}_{2N+s+j}(u_1, \mathfrak{m}_1)\tilde{C}_{2N+s+|\alpha|-j}(u_2, \mathfrak{m}_2) h^N \mathfrak{m}_1 \mathfrak{m}_2$$

uniformly in $u_1 \in S(\mathfrak{m}_1)$*,* $u_2 \in S(\mathfrak{m}_2)$ *and* $h \in (0, 1]$*.*

Proof. We follow arguments from [34, Chapter 7] and [89, Chapters 3 & 4]. Since

$$u_1 \sharp_h u_2 = (e^{i\frac{h}{2}(D_\xi \cdot D_y - D_x \cdot D_\eta)} u_1(x,\xi) u_2(y,\eta))|_{y=x,\eta=\xi} =: (e^{ihA(D)} u_1(x,\xi)u_2(y,\eta))|_{y=x,\eta=\xi}$$

and D^α commutes with $e^{ihA(D)}$ (for any $\alpha \in \mathbb{N}^d$), it suffices to show that there exists $s \in \mathbb{N}$ such that for any $N \in \mathbb{N}$ and order function $\mathfrak{m} : \mathbb{R}^{4d} \to [0, \infty)$,

$$\left| e^{ihA(D)} u(X) - \sum_{j \leq N-1} \frac{(ihA(D))^j}{j!} u(X) \right| \leq C_N \tilde{C}_{2N+s}(u, \mathfrak{m}) h^N \mathfrak{m}(X)$$

uniformly in $u \in S(\mathfrak{m})$ and $h \in (0, 1]$. Here, we use the shorthand $X := (x, y, \xi, \zeta) \in \mathbb{R}^{4d}$.

Since A is non-degenerate, we can let $A^{-1}(X) = \frac{1}{2}\langle Q^{-1}X, X\rangle$ be the dual quadratic form on $\mathbb{R}^{4d}$. Then, as stated in [34, bottom of page 80], $e^{ihA(D)}u = K_h * u$, where

$$K_h(x) = Ch^{-2d} e^{-iA^{-1}(X)/h}.$$

We then write

$$e^{ihA(D)}u = (\chi K_h) * u + ((1-\chi)K_h) * u =: t_1 + t_2,$$

where $\chi \in \mathcal{C}_c^\infty(B(0, 2))$ is equal to 1 in $B(0, 1)$. Set $p := 2d + 1$. By [89, Theorems 3.14 &

4.16 and their proofs], we obtain that

$$\left|t_1(X) - \sum_{j\le N-1} \frac{(ihA(D))^j}{j!}u(X)\right| \le C_N h^N \sum_{|\alpha|\le 2N+p} \sup_{B(X,2)} |\partial^\alpha u|$$
$$\le C_N \tilde{C}_{2N+p}(u,\mathfrak{m})h^N \mathfrak{m}(X).$$

For the second term, we directly apply [34, equation (7.19)] to obtain that for every $k \in \mathbb{N}$,

$$|t_2(X)| \le C_k h^k \sum_{|\alpha|\le k+p} \left\|\langle X-\cdot\rangle^{-k-2d}\partial^\alpha u(\cdot)\right\|_{L^1} \le C_k \tilde{C}_{k+p}(u,\mathfrak{m})h^k \left\|\langle X-\cdot\rangle^{-k-2d}\mathfrak{m}(\cdot)\right\|_{L^1}.$$

Using that $\mathfrak{m}(Y) \le C\langle X-Y\rangle^{N_0}\mathfrak{m}(X)$ for some $N_0 > 0$, it follows that

$$|t_2(X)| \le C_k \tilde{C}_{k+p}(u,\mathfrak{m})h^k \mathfrak{m}(X) \left\|\langle\cdot\rangle^{N_0-k-2d}\right\|_{L^1}.$$

Thus for all $k > N_0 + p$ (so that the above integral is finite),

$$|t_2(X)| \le C_k \tilde{C}_{k+p}(u,m)h^k \mathfrak{m}(X).$$

This completes the result. □

Proposition A.2.2. *There exists $N \in \mathbb{N}$ such that $\|\mathrm{Op}_h(u)\| \le \tilde{C}_N(u,1)$ uniformly in $u \in S(1)$ and $h \in (0,1]$.*

Proof. See [34, Theorem 7.11 and its proof]. □

A.3 Elliptic operators and resolvent estimates

Proposition A.3.1. *Let $\sigma \in ES^m_{1,0}$. Then for all $h \in (0,1]$, the operator $H_h := \mathrm{Op}_h(\sigma)$ is self-adjoint with domain of definition $\mathcal{H}^m$. This means we can define $\mathrm{Op}_h(r_{z,h}) := (z - H_h)^{-1}$ whenever $\Im z \ne 0$. Let $Z \subset \mathbb{C}$ be bounded such that $\Im z \ne 0$ for all $z \in Z$. Then there* *exists $s \in \mathbb{N}$ such that for any $\alpha \in \mathbb{N}^{2d}$,*

$$|\partial^\alpha r_{z,h}(x,\xi)| \leq C_\alpha |\Im z|^{-s-|\alpha|} \langle \xi \rangle^{-m}$$

uniformly in $z \in Z$ and $h \in (0,1]$.

Proof. By [20, Corollary 2 and the paragraph following Theorem 3], we know that H_h is self-adjoint with domain of definition $\mathcal{H}^m$. Applying also [34, the paragraphs between equation (8.11) and Proposition 8.5], it follows that $(i - H_h)^{-1} \in \mathrm{Op}_h(S(\langle \xi, \zeta \rangle^{-m}))$ is a bijection of $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$ onto $\mathcal{H}^m$. For $\Im z \neq 0$, we have that $A_{z,h} := 1 - (i-z)(i-H_h)^{-1}$ is a bijection of $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$ onto itself, with $\left\| A_{z,h}^{-1} \right\| \leq C|\Im z|^{-1}$ uniformly in $z \in Z$. Applying [34, Proposition 8.4] to $\mathrm{Op}_h(b_{z,h}) := A_{z,h}^{-1}$, we obtain that

$$|\partial^\alpha b_{z,h}(x,\xi)| \leq C_\alpha |\Im z|^{-2d-2-|\alpha|}$$

uniformly in $z \in Z$ and $h \in (0,1]$. The result then follows from Proposition A.2.1 (with $N = 0$) and the fact that $(z - H_h)^{-1} = (i - H_h)^{-1} A_{z,h}^{-1}$. □

Below, let $\mathbb{M}_n$ denote the space of Hermitian $n \times n$ matrices.

Proposition A.3.2. *Let $\sigma \in ES^m_{1,0}$ and $\mathcal{W} \subset \mathcal{C}^\infty(\mathbb{R}^{2d}; \mathbb{M}_n)$. Suppose that for any $(\alpha, \beta) \in \mathbb{N}^{2d}$,*

$$|\partial_x^\alpha \partial_\xi^\beta w(x,\xi)| \leq C_\alpha \langle \xi \rangle^{m-|\beta|} \tag{A.3.1}$$

uniformly in $w \in \mathcal{W}$ (meaning that $\mathcal{W} \subset S^m_{1,0}$). For $\mu \in [0,1]$ and $w \in \mathcal{W}$, define $H_{\mu,w} :=$ $\mathrm{Op}(\sigma + \mu w)$. Then there exists $\mu_0 \in (0,1]$ such that the following conditions hold:

1. *If $w \in \mathcal{W}$ and $\mu \in [0, \mu_0]$, then $H_{\mu,w}$ is self-adjoint with domain of definition $\mathcal{H}^m$.*

2. For $\Im z \neq 0$, define $\mathrm{Op}(r_{z,\mu,w}) := (z - H_{\mu,w})^{-1}$*. Let $Z \subset \mathbb{C}$ be bounded such that $\Im z \neq 0$ for all $z \in Z$. Then there exists $s \in \mathbb{N}$ such that for any $\alpha \in \mathbb{N}^{2d}$,*

$$|\partial^\alpha r_{z,\mu,w}(x,\xi)| \leq C_\alpha |\Im z|^{-s-|\alpha|} \langle \xi \rangle^{-m}$$

uniformly in $z \in Z$, $w \in \mathcal{W}$ and $\mu \in [0, \mu_0]$.

Proof. Define $\sigma^{(\mu,w)} := \sigma + \mu w$.

1. The uniform bounds (A.3.1) imply that whenever $\mu > 0$ is sufficiently small, $\sigma^{(\mu,w)} \in ES^m_{1,0}$ for all $w \in \mathcal{W}$. Hence in this case, $H_{\mu,w}$ is self-adjoint with domain of definition $\mathcal{H}^m$.

2. We write $(i - H_{\mu,w})^{-1} = (1 + (i - H_{\mu,w})^{-1} \mu W)(i - H)^{-1}$, which implies

$$(i - H_{\mu,w})^{-1}(1 - \mu W(i - H)^{-1}) = (i - H)^{-1},$$

where $W := \mathrm{Op}_h(w)$ and $H := \mathrm{Op}(\sigma)$. By (A.3.1) and Proposition A.2.2, we conclude that whenever $\mu > 0$ is sufficiently small, $A_{\mu,w} := 1 - \mu W(i - H)^{-1}$ is a bijection of $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$ onto itself, with $A^{-1}_{\mu,w} \in \mathrm{Op}(S(1))$ uniformly in μ and w. Since $(i - H)^{-1} \in \mathrm{Op}(S(\langle \xi \rangle^{-m}))$ by Proposition A.3.1, it follows that $(i - H_{\mu,w})^{-1} \in \mathrm{Op}(S(\langle \xi \rangle^{-m}))$ uniformly in μ and w. The bounds on $r_{z,\mu,w}$ then follow from the same argument that was used in the proof of Proposition A.3.1 (after it was shown that $(i - H_h)^{-1} \in \mathrm{Op}_h(S(\langle \xi, \zeta \rangle^{-m}))$ there).

□

Proposition A.3.3. *Let $\sigma \in ES^m_{1,0}$ and define $H_h := \mathrm{Op}_h(\sigma)$ for $h \in (0,1]$. Let $\phi \in \mathcal{C}^\infty_c(E_1, E_2)$ and define $\mathrm{Op}_h(\nu_h) := \phi(H_h)$. Let $\mathfrak{m} : \mathbb{R}^{2d} \to [0, \infty)$ be any order function such that $\nu_h \in S(\mathfrak{m}^{-\infty})$ and all eigenvalues of σ lie outside the interval (E_1, E_2) whenever $\mathfrak{m}$ is* *sufficiently large. For $z \in \mathbb{C}$, define $\sigma_z := z - \sigma$. For $N \in \mathbb{N}_+$, define $q_{z,h,N}$ recursively by $q_{z,h,1} := \sigma_z^{-1}$ and*

$$q_{z,h,N} = \sigma_z^{-1}\Big(1 - \sum_{j=1}^{N-1}\Big(\frac{(ih(D_\xi \cdot D_y - D_x \cdot D_\eta)/2)^j}{j!}\sigma_z(x,\xi)q_{z,h,N-j}(y,\eta)\Big)|_{y=x,\eta=\xi}\Big)$$

for all $N \geq 2$. Then for all $N \in \mathbb{N}$,

$$\nu_h + \frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\phi}(z) q_{z,h,N} \mathrm{d}^2 z \in S^{-N+1/2}(\mathfrak{m}^{-\infty}). \tag{A.3.2}$$

Proof. Note that $\mathrm{supp}(\tilde{\phi}) \subset (E_1, E_2) \times (-M, M) =: Z$ for some $0 < M < \infty$, hence the integral over $\mathbb{C}$ in (A.3.2) can be restricted to an integral over Z. By assumption, for any $N \in \mathbb{N}$, $z \mapsto q_{z,h,N}$ is analytic in $z \in Z$ so long as $\mathfrak{m}(x,\xi)$ is sufficiently large (independent of h). Integrating by parts, we conclude that $\int_Z \bar{\partial}\tilde{\phi}(z) q_{z,h,N} \mathrm{d}^2 z$ vanishes whenever $\mathfrak{m}(x,\xi)$ is sufficiently large. This implies

$$\nu_h + \frac{1}{\pi}\int_Z \bar{\partial}\tilde{\phi}(z) q_{z,h,N} \mathrm{d}^2 z \in S(\mathfrak{m}^{-\infty}).$$

The result will follow from an h-dependent bound of the above left-hand side and interpolation. Namely, it suffices to show that

$$\nu_h + \frac{1}{\pi}\int_Z \bar{\partial}\tilde{\phi}(z) q_{z,h,N} \mathrm{d}^2 z \in S^{-N+1/4}(1). \tag{A.3.3}$$

By the Helffer-Sjöstrand formula, the above left-hand side equals

$$-\frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\phi}(z) r_{z,h} \mathrm{d}^2 z + \frac{1}{\pi}\int_Z \bar{\partial}\tilde{\phi}(z) q_{z,h,N} \mathrm{d}^2 z = \frac{1}{\pi}\int_Z \bar{\partial}\tilde{\phi}(z)(q_{z,h,N} - r_{z,h}) \mathrm{d}^2 z,$$

where $\mathrm{Op}_h(r_{z,h}) := (z - H_h)^{-1}$. Therefore, given the rapid decay of $\bar{\partial}\tilde{\phi}$ near the real axis, (A.3.3) holds if there exists $s \in \mathbb{N}$ such that for all $\alpha \in \mathbb{N}^d$ and $N \in \mathbb{N}$,

$$|\partial^\alpha (q_{z,h,N} - r_{z,h})| \leq C_{\alpha,N} |\Im z|^{-(2N+2s+|\alpha|+1)} h^N \tag{A.3.4}$$

uniformly in $z \in Z$ and $h \in (0,1]$. We will now prove (A.3.4) by induction.

Using that $\sigma_z \sharp_h r_{z,h} = 1$ for all $h \in (0,1]$, it follows from Proposition A.2.1 that

$$|\partial^\alpha (1 - \sigma_z r_{z,h})| \leq C_{\alpha,1} \sum_{j=0}^{|\alpha|} \tilde{C}_{2+s+j}(\sigma_z, \langle \xi \rangle^m) \tilde{C}_{2+s+|\alpha|-j}(r_{z,h}, \langle \xi \rangle^{-m}) h,$$

hence

$$\begin{aligned} |\partial^\alpha (\sigma_z^{-1} - r_{z,h})| &= |\partial^\alpha (\sigma_z^{-1}(1 - \sigma_z r_{z,h}))| \\ &\leq C_{\alpha,1} \sum_{j=0}^{|\alpha|} \sum_{k=0}^{|\alpha|-j} \tilde{C}_j(\sigma_z^{-1}, \langle \xi \rangle^{-m}) \tilde{C}_{2+s+k}(\sigma_z, \langle \xi \rangle^m) \tilde{C}_{2+s+|\alpha|-j-k}(r_{z,h}, \langle \xi \rangle^{-m}) h \end{aligned}$$

uniformly in $z \in Z$ and $h \in (0,1]$. Observe that for $k \in \mathbb{N}$,

$$\tilde{C}_k(\sigma_z^{-1}, \langle \xi \rangle^{-m}) \leq C |\Im z|^{-1-k}, \qquad \tilde{C}_k(\sigma_z, \langle \xi \rangle^m) \leq C$$

uniformly in $z \in Z$. Since $\tilde{C}_k(r_{z,h}, \langle \xi \rangle^{-m}) \leq C |\Im z|^{-s-k}$ by Proposition A.3.1, we have verified (A.3.4) when $N = 1$.

Now, fix $N \in \mathbb{N}$ and suppose that for all $k \in \{1, \ldots, N\}$,

$$|\partial^\alpha (q_{z,h,k} - r_{z,h})| \leq C_{\alpha,k} |\Im z|^{-(2k+2s+|\alpha|+1)} h^k$$

uniformly in $z \in Z$ and $h \in (0,1]$. Then

$$\begin{aligned}
&q_{z,h,N+1} - r_{z,h} \\
&= \sigma_z^{-1}\Big(1 - \sigma_z r_{z,h} - \sum_{j=1}^{N}\Big(\frac{(ih(D_\xi \cdot D_y - D_x \cdot D_\eta)/2)^j}{j!}\sigma_z(x,\xi) q_{z,h,N+1-j}(y,\eta)\Big)|_{y=x,\eta=\xi}\Big) \\
&= \sigma_z^{-1}\Big(1 - \sum_{j=0}^{N}\Big(\frac{(ih(D_\xi \cdot D_y - D_x \cdot D_\eta)/2)^j}{j!}\sigma_z(x,\xi) r_{z,h}(y,\eta)\Big)|_{y=x,\eta=\xi}\Big) \\
&\quad + \sigma_z^{-1}\sum_{j=1}^{N}\Big(\frac{(ih(D_\xi \cdot D_y - D_x \cdot D_\eta)/2)^j}{j!}\sigma_z(x,\xi)(r_{z,h}(y,\eta) - q_{z,h,N+1-j}(y,\eta))\Big)|_{y=x,\eta=\xi} \\
&=: t_1 + t_2.
\end{aligned}$$

Proposition A.2.1 implies that

$$\begin{aligned}
|\partial^\alpha t_1| &\le C_{\alpha,N+1}\sum_{j=0}^{|\alpha|}\sum_{k=0}^{|\alpha|-j}\tilde{C}_j(\sigma_z^{-1},\langle\xi\rangle^{-m})\tilde{C}_{2(N+1)+s+k}(\sigma_z,\langle\xi\rangle^m) \\
&\qquad\qquad \times \tilde{C}_{2(N+1)+s+|\alpha|-j-k}(r_{z,h},\langle\xi\rangle^{-m})h^{N+1} \\
&\le C_{\alpha,N+1}|\Im z|^{-(2(N+1)+2s+|\alpha|+1)}h^{N+1}.
\end{aligned}$$

Define $t_2 =: \sigma_z^{-1}\sum_{j=1}^{N} t_{2,j}$. By our inductive hypothesis,

$$\begin{aligned}
|\partial^\alpha t_{2,j}| &\le C_{\alpha,j}h^j\sum_{i=0}^{|\alpha|+j}\tilde{C}_i(\sigma_z,\langle\xi\rangle^m)\tilde{C}_{|\alpha|+j-i}(r_{z,h} - q_{z,h,N+1-j},1)\langle\xi\rangle^m \\
&\le C_{\alpha,j}|\Im z|^{-(2(N+1-j)+2s+|\alpha|+j+1)}h^{N+1}\langle\xi\rangle^m \\
&= C_{\alpha,j}|\Im z|^{-(2(N+1)+2s+|\alpha|+1-j)}h^{N+1}\langle\xi\rangle^m \\
&\le C_{\alpha,j}|\Im z|^{-(2(N+1)+2s+|\alpha|)}h^{N+1}\langle\xi\rangle^m.
\end{aligned}$$

It follows that

$$|\partial^\alpha(\sigma_z^{-1}t_{2,j})| \le C_{\alpha,j}|\Im z|^{-(2(N+1)+2s+|\alpha|+1)}h^{N+1}.$$

for all $j \in \{1,\dots,N\}$. We have thus verified (A.3.4) for all $N \in \mathbb{N}$, and the proof is complete. $\square$

For completeness, we now write an expansion for ν_h that does not involve an integral.

Proposition A.3.4. *Take σ, ν_h, φ and m as above. Let $\{\mu_j\}_{j=1}^d$ denote the eigenvalues of σ and $\{\Pi_j\}_{j=1}^d$ the corresponding eigenprojections, so that $\sigma = \sum_{j=1}^d \mu_j \Pi_j$. Then*

$$\nu_h = \varphi'(\sigma) + ih \sum_{\ell_1,\ell_2,\ell_3=1}^{d} \Psi(\mu_{\ell_1},\mu_{\ell_2},\mu_{\ell_3})\Pi_{\ell_1} \sum_{k=1}^{n} (\partial_{x_k}\sigma\Pi_{\ell_2}\partial_{\xi_k}\sigma - \partial_{\xi_k}\sigma\Pi_{\ell_2}\partial_{x_k}\sigma)\Pi_{\ell_3} + O(h^{3/2})$$

in $S(m^{-\infty})$, where $\Psi \in \mathcal{C}^\infty(\mathbb{R}^3)$ is defined by

$$\Psi(x,y,z) = \frac{1}{(x-y)(x-z)}\varphi'(x) + \frac{1}{(y-x)(y-z)}\varphi'(y) + \frac{1}{(z-x)(z-y)}\varphi'(z).$$

Proof. This result is a direct application of Proposition A.3.3. Namely, $q_{z,h,1} = \sigma_z^{-1}$, so the $O(1)$ in the expansion for ν_h is

$$-\frac{1}{\pi}\int_{\mathbb{C}} \bar\partial\tilde{\varphi}'(z)\sigma_z^{-1}\,\mathrm{d}^2 z = \varphi'(\sigma).$$

The $O(h)$ term is

$$-\frac{i}{\pi}\int_{\mathbb{C}} \bar\partial\tilde{\varphi}'(z)\sigma_z^{-1}\{\sigma_z,\sigma_z^{-1}\}\mathrm{d}^2 z.$$

Using the eigendecomposition $\sigma = \sum_{j=1}^{d} \mu_j \Pi_j$, a simple calculation reveals that

$$\sigma_z^{-1}\{\sigma_z, \sigma_z^{-1}\} =$$
$$\sum_{\ell_1,\ell_2,\ell_3=1}^{d} (z-\mu_{\ell_1})^{-1}(z-\mu_{\ell_2})^{-1}(z-\mu_{\ell_3})^{-1}\Pi_{\ell_1}\sum_{k=1}^{n}(\partial_{x_k}\sigma\Pi_{\ell_2}\partial_{\xi_k}\sigma - \partial_{\xi_k}\sigma\Pi_{\ell_2}\partial_{x_k}\sigma)\Pi_{\ell_3}.$$

The result then follows from the identity

$$-\frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\varphi}'(z)(z-\mu_{\ell_1})^{-1}(z-\mu_{\ell_2})^{-1}(z-\mu_{\ell_3})^{-1}\mathrm{d}^2 z = \Psi(\mu_{\ell_1}, \mu_{\ell_2}, \mu_{\ell_3}).$$

$\square$

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