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PEIERLS SUBSTITUTION FOR MAGNETIC BLOCH BANDS

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We consider the one-particle Schrödinger operator in two dimensions with a periodic potential and a strong constant magnetic field perturbed by slowly varying, nonperiodic scalar and vector potentials $\phi(\varepsilon x)$ and $A(\varepsilon x)$ for $\varepsilon \ll 1$. For each isolated family of magnetic Bloch bands we derive an effective Hamiltonian that is unitarily equivalent to the restriction of the Schrödinger operator to a corresponding almost invariant subspace. At leading order, our effective Hamiltonian can be interpreted as the Peierls substitution Hamiltonian widely used in physics for nonmagnetic Bloch bands. However, while for nonmagnetic Bloch bands the corresponding result is well understood, both on a heuristic and on a rigorous level, for magnetic Bloch bands it is not clear how to even define a Peierls substitution Hamiltonian beyond a formal expression. The source of the difficulty is a topological obstruction: in contrast to the nonmagnetic case, magnetic Bloch bundles are generically not trivializable. As a consequence, Peierls substitution Hamiltonians for magnetic Bloch bands turn out to be pseudodifferential operators acting on sections of nontrivial vector bundles over a two-torus, the reduced Brillouin zone. Part of our contribution is the construction of a suitable Weyl calculus for such pseudodifferential operators.

As an application of our results we construct a new family of canonical one-band Hamiltonians $H^B_{\theta,q}$ for magnetic Bloch bands with Chern number $\theta \in \mathbb{Z}$ that generalizes the Hofstadter model $H^B_{\mathrm{Hof}} = H^B_{0,1}$ for a single nonmagnetic Bloch band. It turns out that $H^B_{\theta,q}$ is isospectral to $H^{q^2 B}_{\mathrm{Hof}}$ for any θ and all spectra agree with the Hofstadter spectrum depicted in his famous (black and white) butterfly. However, the resulting Chern numbers of subbands, corresponding to Hall conductivities, depend on θ and q, and thus the models lead to different colored butterflies.

1. Introduction

We consider perturbations of the self-adjoint Schrödinger operator

$$H_{B_0,\Gamma} = \tfrac{1}{2}(-\mathrm{i}\nabla_x - A_0)^2 + V_\Gamma,$$

densely defined on $L^2(\mathbb{R}^2)$, where $A_0 : \mathbb{R}^2 \to \mathbb{R}^2$ and $V_\Gamma : \mathbb{R}^2 \to \mathbb{R}$ act as multiplication operators. Here $A_0(x) = (-B_0 x_2, 0)$ is the vector potential of a constant magnetic field $B_0 \in \mathbb{R}$ and the scalar potential V_Γ is assumed to be periodic with respect to a Bravais lattice $\Gamma \subset \mathbb{R}^2$. The spectral properties of the operator $H_{B_0,\Gamma}$ are extremely sensitive to the relation between the numerical value of $B_0 \in \mathbb{R}$ and the area $|\Gamma|$ of one lattice cell. When B_0 and Γ are commensurable, in the sense that $B_0|\Gamma|/2\pi = p/q \in \mathbb{Q}$, the operator $H_{B_0,\Gamma}$ is unitarily equivalent by an explicit unitary transformation $\mathscr{F}_q$ to a countable direct sum of multiplication operators by real-valued continuous functions $E_n : \mathbb{T}^*_q \to \mathbb{R}$ with $E_n(k) \le E_{n+1}(k)$

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for all $k \in \mathbb{T}_q^*$ and $n \in \mathbb{N} = \{1, 2, \dots\}$. Here the two-dimensional torus $\mathbb{T}_q^*$ is the Pontryagin dual of a subgroup Γ_q of Γ. In summary, it holds that

$$\widehat{H}_{B_0,\Gamma} := \mathcal{F}_q H_{B_0,\Gamma} \mathcal{F}_q^* = \sum_{n=1}^{\infty} E_n P_n \quad \text{on } \mathcal{H} := \mathcal{F}_q L^2(\mathbb{R}^3) = L^2(\mathbb{T}_q^*; \mathcal{H}_{\mathrm{f}}) \cong \bigoplus_{n=1}^{\infty} L^2(\mathbb{T}_q^*), \tag{1}$$

where P_n is the orthogonal projection onto the n-th summand in the direct sum. As a consequence, the spectrum $\sigma(H_{B_0,\Gamma}) = \bigcup_{n=1}^{\infty} E_n(\mathbb{T}_q^*)$ is a union of intervals and purely absolutely continuous. If, on the other hand, $B_0|\Gamma|/2\pi \notin \mathbb{Q}$, then it is expected that $\sigma(H_{B_0,\Gamma})$ is a set of Cantor type, i.e., a closed nowhere-dense set of zero Lebesgue measure. The proof of this so-called ten martini problem was given only recently [Avila and Jitomirskaya 2009] and it only applies to simple tight-binding models on $\ell^2(\mathbb{Z}^2)$. The most prominent picture of this commensurability problem is the fractal Hofstadter butterfly, a plot of the spectrum of such a simple tight binding model as a function of the magnetic field B_0; see Figure 2 in Section 7.

The physical meaning of the operator $H_{B_0,\Gamma}$ is that of a Hamiltonian for a single particle constrained to move in a planar two-dimensional crystalline lattice under the influence of a constant magnetic field of strength B_0 perpendicular to the plane. However, from the point of view of physical applications and experiments, a constant magnetic field B_0 is a highly idealized situation that can be realized only approximately. The distinction between rational and irrational magnetic fields B_0 is a purely mathematical one. Thus it is of genuine interest to understand perturbations of $H_{B_0,\Gamma}$ by potentials $A^\varepsilon(x) := A(\varepsilon x)$ and $\Phi^\varepsilon(x) := \Phi(\varepsilon x)$ corresponding to magnetic and electric fields $B^\varepsilon(x) := \varepsilon(\operatorname{curl} A)(\varepsilon x)$ and $\mathcal{E}^\varepsilon(x) := \varepsilon(\nabla\Phi)(\varepsilon x)$ that are small and slowly varying in the asymptotic limit $\varepsilon \ll 1$. Here $A : \mathbb{R}^2 \to \mathbb{R}^2$ and $\Phi : \mathbb{R}^2 \to \mathbb{R}$ are smooth functions. We therefore consider the self-adjoint Schrödinger operator

$$H^\varepsilon_{B_0,\Gamma} = \tfrac{1}{2}(-\mathrm{i}\nabla_x - A_0 - A^\varepsilon)^2 + V_\Gamma + \Phi^\varepsilon$$

for a fixed rational value of $B_0|\Gamma|/2\pi = p/q$ in the asymptotic limit $\varepsilon \ll 1$ as a perturbation of the simple block structure (1). It follows by well-known techniques of adiabatic perturbation theory that parts of the block decomposition (1) are stable under such perturbations: Assuming, for example, for a single function E_n the gap condition $E_{n-1}(k) < E_n(k) < E_{n+1}(k)$ for all $k \in \mathbb{T}_q^*$, one can construct from P_n an orthogonal projection Π_n^ε such that $\|[\Pi_n^\varepsilon, \widehat{H}^\varepsilon_{B_0,\Gamma}]\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon^\infty)$. While the restriction $P_n \widehat{H}_{B_0,\Gamma} P_n$ of the unperturbed operator to one of its invariant subspaces ran P_n acts as multiplication by the function E_n, the restriction $\Pi_n^\varepsilon \widehat{H}^\varepsilon_{B_0,\Gamma} \Pi_n^\varepsilon$ of the perturbed operator $\widehat{H}^\varepsilon_{B_0,\Gamma}$ to one of its almost invariant subspaces ran Π_n^ε a priori has no simple form. The "Peierls substitution rule", widely used in physics, suggests that $\Pi_n^\varepsilon \widehat{H}^\varepsilon_{B_0,\Gamma} \Pi_n^\varepsilon$ is unitarily equivalent to a pseudodifferential operator with principal part

$$E_n(k - A(\mathrm{i}\varepsilon\nabla_k)) + \Phi(\mathrm{i}\varepsilon\nabla_k)$$

acting on some space of functions on the torus $\mathbb{T}_q^*$. The main result of our paper is to turn this claim into a precise statement and to prove it: we show that the blocks $\Pi_n^\varepsilon \widehat{H}^\varepsilon_{B_0,\Gamma} \Pi_n^\varepsilon$ of the perturbed operator are unitarily equivalent to pseudodifferential operators acting on spaces of sections of possibly nontrivial vector bundles over the torus with principal part given by the Peierls substitution rule. A special case of our main result, Theorem 5.1, is the following statement:

Theorem 1.1. *Let A, Φ be smooth bounded functions with bounded derivatives of any order and $B_0|\Gamma|/2\pi = p/q \in \mathbb{Q}$. For any simple Bloch function E_n of the unperturbed Hamiltonian $H_{B_0,\Gamma}$ satisfying the gap condition, there exist for $\varepsilon > 0$ small enough*

- *an orthogonal projection Π_n^ε,*
- *a line bundle Ξ_θ over the torus $\mathbb{T}_q^*$ with connection ∇^θ and Chern number $\theta \in \mathbb{Z}$,*
- *a unitary map $U^\varepsilon : \operatorname{ran} \Pi_n^\varepsilon \to L^2(\Xi_\theta)$, and*
- *a pseudodifferential operator $E_n^\varepsilon \in \mathcal{L}(L^2(\Xi_\theta))$ with*

$$\left\| E_n^\varepsilon - \left(E_n(k - A(\mathrm{i}\varepsilon\nabla_k^\theta)) + \Phi(\mathrm{i}\varepsilon\nabla_k^\theta) \right) \right\|_{\mathcal{L}(L^2(\Xi_\theta))} = \mathcal{O}(\varepsilon)$$

such that $\|[\Pi_n^\varepsilon, \widehat{H}_{B_0,\Gamma}^\varepsilon]\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon^\infty)$ and

$$\|U^\varepsilon \Pi_n^\varepsilon \widehat{H}_{B_0,\Gamma}^\varepsilon \Pi_n^\varepsilon U^{\varepsilon *} - E_n^\varepsilon\|_{\mathcal{L}(L^2(\Xi_\theta))} = \mathcal{O}(\varepsilon^\infty). \tag{2}$$

In Theorem 5.1 we actually consider a more general situation, where a single band E_n is replaced by a finite family of bands. Then Ξ_θ becomes a vector bundle of finite rank and the Peierls substitution Hamiltonian is a pseudodifferential operator with matrix-valued symbol. We also compute the subprincipal symbol of E_n^ε explicitly, which contains important information for transport and magnetic properties of electron gases in periodic media.

Theorem 5.1, and its special case Theorem 1.1, were shown before for the case $B_0 = 0$ [Panati et al. 2003a]. There one has $\theta = 0$ and Ξ_0 is a trivial vector bundle over the torus $\mathbb{T}_q^*$. For the case $B_0 \neq 0$, the validity and the meaning of Peierls substitution, even on a purely heuristic level, were a matter of debate (see, e.g., [Zak 1986; 1991]) and, to our knowledge, not even a precise conjecture was stated in the literature.

Before giving more details, let us mention that the systematic or even rigorous analysis of two-dimensional systems with periodic potential and magnetic field is a continuing theme in theoretical physics, for example [Peierls 1933; Blount 1962; Zak 1968; Hofstadter 1976; Thouless et al. 1982; Sundaram and Niu 1999; Gat and Avron 2003b], and also in mathematical physics and mathematics, for example [Dubrovin and Novikov 1980a; 1980b; Novikov 1981; Buslaev 1987; Bellissard 1988; Guillot et al. 1988; Helffer and Sjöstrand 1989; Rammal and Bellissard 1990; Helffer et al. 1990; Helffer and Sjöstrand 1990a; 1990b; Nenciu 1991; Gérard et al. 1991; Hövermann et al. 2001; Panati et al. 2003a; Dimassi et al. 2004; Panati 2007; Avila and Jitomirskaya 2009; De Nittis and Panati 2010; De Nittis and Lein 2011; Stiepan and Teufel 2013]. We can mention here only a small part of the enormous literature and we refer to [Nenciu 1991] for a review of the mathematical and physical literature to that point.

Most of the mathematical literature is concerned with the problem of recovering the spectrum and sometimes the density of states of the perturbed Hamiltonian $H_{B_0,\Gamma}^\varepsilon$. In some cases this is done by constructing isospectral effective Hamiltonians in the spirit of the Peierls substitution rule; see, e.g., [Rammal and Bellissard 1990; Helffer et al. 1990; Helffer and Sjöstrand 1989; 1990a; 1990b; Gérard et al. 1991]. With a few exceptions, most notably [Rammal and Bellissard 1990], the limiting cases $B_0 = 0$ and $B_0 \to \infty$ were considered. More recently, the question of constructing unitarily equivalent effective Hamiltonians was taken up in [Panati et al. 2003a; De Nittis and Panati 2010; De Nittis and Lein 2011] and the limiting regimes $B_0 = 0$ and $B_0 \to \infty$ are fully understood by now even on a mathematical level. For a thorough discussion of the question of why unitary equivalence is important also from a physics point of view, we refer to [De Nittis and Panati 2010]. Let us mention here only one example: The two canonical models for effective Hamiltonians for the asymptotic regimes $B_0 = 0$ and $B_0 \to \infty$ are exactly isospectral. This is known as the duality of the Hofstadter model; see, e.g., [Gat and Avron 2003a]. However, they are not unitarily equivalent and describe different physics.

The problem of constructing unitarily equivalent effective Hamiltonians in the intermediate regime of finite $B_0 \neq 0$ was, to our knowledge, completely open up to now[1] and its solution is the main content of our paper. While we use the same basic approach that was applied in [Panati et al. 2003a; De Nittis and Panati 2010] for the cases $B_0 = 0$ and $B_0 \to \infty$, namely adiabatic perturbation theory [Panati et al. 2003b], there is a major geometric obstruction in extending these methods to perturbations around finite values of B_0 such that $B_0|\Gamma|/2\pi = p/q \in \mathbb{Q}$, which we briefly explain. In all cases the projections P_n in (1) act on $L^2(\mathbb{T}^*_q, \mathcal{H}_{\mathrm{f}})$ fiberwise, that is, they are given by projection-valued functions $P_n : \mathbb{T}^*_q \to \mathcal{L}(\mathcal{H}_{\mathrm{f}}),\ k \mapsto P_n(k)$. For an isolated simple band E_n the corresponding projection-valued function $P_n(\,\cdot\,)$ is smooth and defines a complex line bundle over $\mathbb{T}^*_q$, the so-called Bloch bundle associated with the Bloch band E_n. For $B_0 = 0$ the Bloch bundles are trivial and the effective operator E^ε_n is a pseudodifferential operator acting on $L^2(\mathbb{T}^*_1)$, the space of L^2-sections of the trivial line bundle over the torus $\mathbb{T}^*_1$. The Bloch bundles for $B_0 \neq 0$ are not trivial in general and E^ε_n has to be understood as a pseudodifferential operator acting on the sections of a nontrivial line bundle Ξ_θ over the torus $\mathbb{T}^*_q$.

An important shortcoming of our result is, however, that we cannot allow for the case of a perturbation by a constant magnetic field B, corresponding to a linear vector potential A, in all steps of the derivation. While an (almost) invariant subspace and the corresponding (almost) block structure of the perturbed Hamiltonian can still be established in this case, and also the effective Hamiltonian $\mathrm{Op}^\theta(E_n(k - A(r)) + \Phi(r))$ remains well defined for linear A, the unitary map intertwining the (almost) invariant subspace and the reference space, as we construct it, no longer exists. For $\theta = 0$ this problem actually disappears, and we recover the results for nonmagnetic Bloch bands with constant small magnetic fields B obtained in [De Nittis and Panati 2010; De Nittis and Lein 2011]. Note, however, that the physically relevant situation where B and also $E = -\nabla\Phi$ are constant over a macroscopic volume containing ε^{-2} lattice sites is included in all of our results.

Let us mention that some of the physically relevant questions can be answered without establishing Peierls substitution in our sense of unitary equivalence. There are, in particular, semiclassical and algebraic approaches that allow for direct computation of many relevant quantities without the detour via Peierls substitution. The modified semiclassical equations of motion for magnetic Bloch bands [Sundaram and Niu 1999] became the starting point for a large number of quantitative results; see, e.g., [Xiao et al.

[1] It was observed in [Dimassi et al. 2004] that the method of [Panati et al. 2003a] can be directly applied also to magnetic Bloch bands if one assumes that the magnetic Bloch bundles are trivial. But this assumption is generically not satisfied.

2010] and references therein. This approach was rigorously derived and extended in [Stiepan and Teufel 2013; Teufel 2012]. In [Gat and Avron 2003b] the authors apply Bohr–Sommerfeld quantization with phases modified by the Berry curvature and the Rammal–Wilkinson term in order to compute the orbital magnetization in the Hofstadter model. For the case where B is constant or periodic and $\Phi = 0$, the algebraic approach of Bellissard and coworkers [Bellissard 1988; Rammal and Bellissard 1990; Bellissard et al. 1991] provides a powerful tool for expansions to all orders for eigenvalues, free energies and quantities derived from there. This approach can also cope with random perturbations and has developed into a very general machinery; see, e.g., [Bellissard et al. 1994; Schulz-Baldes and Teufel 2013] and references therein.

We end the introduction with a short outline of the paper. In Section 2 we give a precise formulation of the setup and introduce all relevant quantities and assumptions. In Section 3 we briefly formulate the result on the existence and the construction of almost invariant subspaces. We do not give a proof here, since nothing interesting changes with respect to the nonmagnetic case at this point. In Section 4 we analyze in detail the structure of magnetic Bloch bundles. As a result we can construct the reference space for the effective Hamiltonian and the unitary map from the almost invariant subspace to this reference space. This analysis is one key ingredient of our main result, which we formulate and prove in Section 5. The result and its proof are based on geometric Weyl calculi for operators acting on sections of nontrivial vector bundles, the other key ingredients, which are developed in Section 6. In the final Section 7, we explicitly compute Peierls substitution Hamiltonians for magnetic subbands of the Hofstadter Hamiltonian. The Hofstadter model is the canonical model for a single nonmagnetic Bloch band perturbed by a constant magnetic field B_0. As a result we find a new two-parameter family $H^B_{\theta,q}$ (see (32)) of Hofstadter-like Hamiltonians indexed by integers $\theta \in \mathbb{Z}$ and $q \in \mathbb{N}$. The operator $H^B_{\theta,q}$ can be viewed as the canonical model for a magnetic Bloch band with Chern number θ and originating from a Bloch band split into q magnetic subbands. Like the Hofstadter model itself, all $H^B_{\theta,q}$ are representations of an element of the noncommutative torus algebra, the abstract Hofstadter operator. As a consequence they are all isospectral and lead to the same black and white butterfly, Figure 2. But the transport properties encoded in the Chern numbers of spectral bands depend on θ and q and they give rise to different colored butterflies; see Figure 4. The results of Section 7 and a more detailed analysis presented in [Amr et al. 2015] suggest that our main theorem, Theorem 5.1, also holds for perturbations by magnetic fields with potentials A of linear growth.

2. Perturbed periodic and magnetic Schrödinger operators

We consider perturbations of a one-particle Schrödinger operator with a periodic potential and a constant magnetic field in two dimensions. The unperturbed operator is given by

$$H_{\mathrm{MB}} = \tfrac{1}{2}(-\mathrm{i}\nabla_x - A^{(0)}(x))^2 + V_{\widetilde{\Gamma}}(x)$$

with domain $H^2_{A^{(0)}}(\mathbb{R}^2)$, a magnetic Sobolev space. Here

$$A^{(0)}(x) := \mathcal{B}_0 x \quad \text{with} \quad \mathcal{B}_0 := \begin{pmatrix} 0 & -B_0 \\ 0 & 0 \end{pmatrix}$$

and $V_{\widetilde{\Gamma}}$ is periodic with respect to a Bravais lattice

$$\widetilde{\Gamma} := \{a\tilde{\gamma}_1 + b\tilde{\gamma}_2 \in \mathbb{R}^2 \mid a, b \in \mathbb{Z}\}$$

spanned by a basis $(\tilde{\gamma}_1, \tilde{\gamma}_2)$ of $\mathbb{R}^2$, i.e., $V_{\widetilde{\Gamma}}(x+\tilde{\gamma}) = V_{\widetilde{\Gamma}}(x)$ for all $\tilde{\gamma} \in \widetilde{\Gamma}$. We will later assume that $B_0 \in \mathbb{R}$ satisfies a commensurability condition, so that H_{MB} obtains a magnetic Bloch band structure.

The full Hamiltonian is a perturbation of H_{MB} by "small" magnetic and electric fields of order ε. More precisely, let $A^{(1)}$ be a linear vector potential of an additional constant magnetic field B_1 and let $A^{(2)}$ and Φ be bounded vector and scalar potentials; then the full Hamiltonian H^ε reads

$$H^\varepsilon = \tfrac{1}{2}(-\mathrm{i}\nabla_x - A^{(0)}(x) - \varepsilon A^{(1)}(x) - A^{(2)}(\varepsilon x))^2 + V_{\widetilde{\Gamma}}(x) + \Phi(\varepsilon x) \tag{3}$$

with domain $H^2_{A^{(0)}+\varepsilon A^{(1)}}(\mathbb{R}^2)$, where

$$H^m_A := \{f \in L^2(\mathbb{R}^2) \mid (\mathrm{i}\nabla_x + A(x))^\alpha f \in L^2(\mathbb{R}^2) \text{ for all } \alpha \in \mathbb{N}_0^2 \text{ with } |\alpha| \le m\}$$

and $\mathbb{N}_0 = \{0, 1, 2, \dots\}$.

Assumption 1. *Assume that $A^{(2)} \in C_{\mathrm{b}}^\infty(\mathbb{R}^2, \mathbb{R}^2)$ satisfies the gauge condition $A^{(2)}(x)\cdot\tilde{\gamma}_2 = 0$ for all $x \in \mathbb{R}^2$ and that $\Phi \in C_{\mathrm{b}}^\infty(\mathbb{R}^2, \mathbb{R})$. Let $V_{\widetilde{\Gamma}} : \mathbb{R}^2 \to \mathbb{R}$ be a measurable function such that $V_{\widetilde{\Gamma}}(x+\tilde{\gamma}) = V_{\widetilde{\Gamma}}(x)$ for all $\tilde{\gamma} \in \widetilde{\Gamma}$ and that the operator of multiplication by $V_{\widetilde{\Gamma}}$ is relatively $(-\mathrm{i}\nabla - A^{(0)} - \varepsilon A^{(1)})^2$-bounded with relative bound smaller than 1 for all $\varepsilon > 0$ small enough.*

Under these conditions, H_{MB} and H^ε are essentially self-adjoint on $C_0^\infty(\mathbb{R}^2)$, and self-adjoint on $H^2_{A^{(0)}}(\mathbb{R}^2)$ and $H^2_{A^{(0)}+\varepsilon A^{(1)}}(\mathbb{R}^2)$, respectively. Note that any $V_{\widetilde{\Gamma}} \in L^2_{\mathrm{loc}}(\mathbb{R}^2)$ satisfies Assumption 1.

The band structure of H_{MB}. The magnetic translation of functions on $\mathbb{R}^2$ by $\tilde{\gamma}_j$ is defined by

$$(\widetilde{T}_j \psi)(x) := \mathrm{e}^{\mathrm{i}\langle x, \mathcal{B}_0 \tilde{\gamma}_j\rangle} \psi(x - \tilde{\gamma}_j). \tag{4}$$

On $L^2(\mathbb{R}^2)$ the magnetic translations are unitary and leave invariant the magnetic momentum operator and the periodic potential:

$$\widetilde{T}_j^{-1}(-\mathrm{i}\nabla - A^{(0)})\widetilde{T}_j = (-\mathrm{i}\nabla - A^{(0)}) \quad \text{and} \quad \widetilde{T}_j^{-1} V_{\widetilde{\Gamma}} \widetilde{T}_j = V_{\widetilde{\Gamma}}, \quad \text{and thus} \quad \widetilde{T}_j^{-1} H_{\mathrm{MB}} \widetilde{T}_j = H_{\mathrm{MB}}.$$

Because

$$\widetilde{T}_1 \widetilde{T}_2 = \mathrm{e}^{\mathrm{i}\langle \tilde{\gamma}_2, \mathcal{B}_0 \tilde{\gamma}_1\rangle} \widetilde{T}_2 \widetilde{T}_1,$$

we only obtain a unitary representation of $\widetilde{\Gamma}$ if $\langle \tilde{\gamma}_2, \mathcal{B}_0 \tilde{\gamma}_1\rangle \in 2\pi\mathbb{Z}$. Here $\langle \tilde{\gamma}_2, \mathcal{B}_0 \tilde{\gamma}_1\rangle = B_0 \tilde{\gamma}_1 \wedge \tilde{\gamma}_2$ is the magnetic flux through the unit cell M of the lattice Γ with oriented volume $\tilde{\gamma}_1 \wedge \tilde{\gamma}_2$.

Assumption 2. *The flux of B_0 per unit cell satisfies $\langle \tilde{\gamma}_2, \mathcal{B}_0 \tilde{\gamma}_1\rangle = 2\pi p/q \in 2\pi\mathbb{Q}$.*

By passing to the sublattice $\Gamma \subset \widetilde{\Gamma}$ spanned by the basis $(\gamma_1, \gamma_2) := (q\tilde{\gamma}_1, \tilde{\gamma}_2)$ and defining the magnetic translations T_1 and T_2 analogously, we achieve $\langle \gamma_2, \mathcal{B}_0 \gamma_1 \rangle = 2\pi p \in 2\pi\mathbb{Z}$. Hence

$$T : \Gamma \to \mathcal{L}(L^2(\mathbb{R}^2)), \quad \gamma = n_1\gamma_1 + n_2\gamma_2 \mapsto T_\gamma := T_1^{n_1} T_2^{n_2}, \tag{5}$$

is a unitary representation of Γ on $L^2(\mathbb{R}^2)$ satisfying

$$T_\gamma^{-1} H_{\mathrm{MB}} T_\gamma = H_{\mathrm{MB}} \tag{6}$$

for all $\gamma \in \Gamma$. Before we introduce the Bloch–Floquet transformation in order to exploit the translation invariance of H_{MB}, we first define a number of useful function spaces. Let

$$\mathcal{H}_{\mathrm{f}} := \{ f \in L^2_{\mathrm{loc}}(\mathbb{R}^2) \mid T_\gamma f = f \ \text{ for all } \ \gamma \in \Gamma \},$$

which, equipped with the inner product $\langle f, g \rangle_{\mathcal{H}_{\mathrm{f}}} := \int_M \overline{f(y)} g(y)\, \mathrm{d}y$, is a Hilbert space. Analogously, for $m \in \mathbb{N}$,

$$\mathcal{H}^m_{A^{(0)}}(\mathbb{R}^2) := \{ f \in \mathcal{H}_{\mathrm{f}} \mid (-\mathrm{i}\nabla - A^{(0)})^\alpha f \in \mathcal{H}_{\mathrm{f}} \ \text{ for all } \ \alpha \in \mathbb{N}_0^2 \ \text{ with } \ |\alpha| \le m \}$$

is a Hilbert space with inner product

$$\langle f, g \rangle_{\mathcal{H}^m_{A^{(0)}}(\mathbb{R}^2)} := \sum_{|\alpha| \le m} \langle (-\mathrm{i}\nabla - A^{(0)})^\alpha f, (-\mathrm{i}\nabla - A^{(0)})^\alpha g \rangle_{\mathcal{H}_{\mathrm{f}}}.$$

Let Γ^* be the dual lattice of Γ, i.e., the $\mathbb{Z}$-span of the unique basis (γ_1^*, γ_2^*) such that $\gamma_i^* \cdot \gamma_j = 2\pi\delta_{ij}$. By M and M^* we denote the centered fundamental cells of Γ and Γ^*, respectively. On $\mathcal{H}_{\mathrm{f}}$ a unitary representation of the dual lattice Γ^* is given by

$$\tau : \Gamma^* \to \mathcal{L}(\mathcal{H}_{\mathrm{f}}), \quad \gamma^* \mapsto \tau(\gamma^*) \quad \text{with} \quad (\tau(\gamma^*)f)(y) := \mathrm{e}^{\mathrm{i}y\cdot\gamma^*} f(y).$$

Finally, let the space of τ-equivariant functions be

$$\mathcal{H}_\tau := \{ f \in L^2_{\mathrm{loc}}(\mathbb{R}^2_k, \mathcal{H}_{\mathrm{f}}) \mid f(k - \gamma^*) = \tau(\gamma^*) f(k) \ \text{ for all } \ \gamma^* \in \Gamma^* \}$$

equipped with the inner product $\langle f, g \rangle_{\mathcal{H}_\tau} = \int_{M^*} \langle f(k), g(k) \rangle_{\mathcal{H}_{\mathrm{f}}}\, \mathrm{d}k$, where $\mathrm{d}k$ is the normalized Lebesgue measure on M^* and $\mathcal{H}_\tau$ is a Hilbert space.

For $\psi \in C_0^\infty(\mathbb{R}^2)$, the magnetic Bloch–Floquet transformation is defined by

$$(\mathcal{U}_{\mathrm{BF}}\psi)(k, y) := \sum_{\gamma \in \Gamma} \mathrm{e}^{-\mathrm{i}(y-\gamma)\cdot k} (T_\gamma \psi)(y). \tag{7}$$

It extends uniquely to a unitary mapping $\mathcal{U}_{\mathrm{BF}} : L^2(\mathbb{R}^2) \to \mathcal{H}_\tau$ and its inverse is given by

$$(\mathcal{U}_{\mathrm{BF}}^{-1}\phi)(x) = \int_{M^*} \mathrm{e}^{\mathrm{i}k\cdot x} \phi(k, x)\, \mathrm{d}k.$$

Because of (6) the operator H_{MB} fibers in the magnetic Bloch–Floquet representation as

$$H^0_{\mathrm{BF}} := \mathcal{U}_{\mathrm{BF}} H_{\mathrm{MB}} \mathcal{U}_{\mathrm{BF}}^* = \int_{M^*}^{\oplus} H_{\mathrm{per}}(k)\, \mathrm{d}k,$$

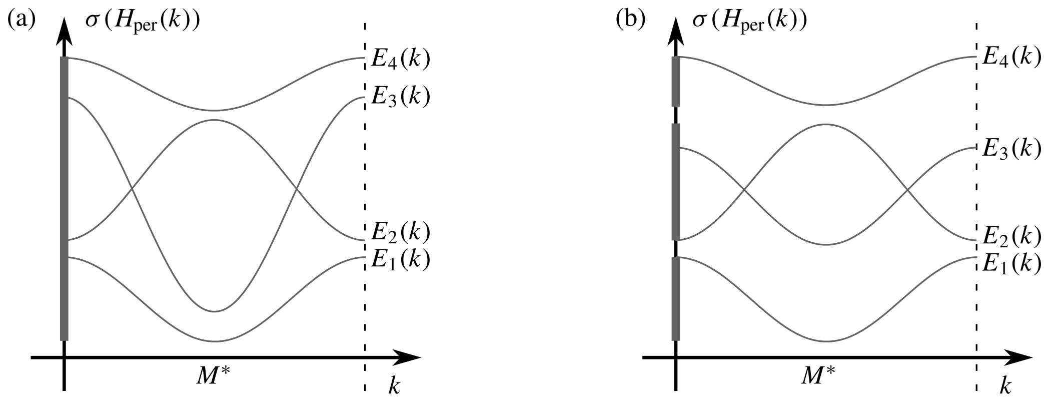

Figure 1. Two sketches of Bloch bands. Note that $k \in \mathbb{R}^2$, so the graphs of the Bloch bands are really surfaces. In (a) the families $\{E_1(k)\}$, $\{E_2(k), E_3(k)\}$ and $\{E_4(k)\}$ are all isolated, but none of them is strictly isolated. In (b) they are all strictly isolated.

where

$$H_{\rm per}(k) := \tfrac{1}{2}(-\mathrm{i}\nabla_y - A^{(0)}(y) + k)^2 + V_\Gamma(y)$$

acts for any fixed $k \in M^*$ on the k-independent domain $\mathcal{H}^2_{A^{(0)}}(\mathbb{R}^2) \subset \mathcal{H}_{\rm f}$. The domain $H^2_{A^{(0)}}(\mathbb{R}^2)$ of $H_{\rm MB}$ is mapped to

$$\mathcal{U}_{\mathcal{F}} H^2_{A^{(0)}}(\mathbb{R}^2) =: L^2_\tau(\mathbb{R}^2, \mathcal{H}^2_{A^{(0)}}(\mathbb{R}^2)) = L^2_{\rm loc}(\mathbb{R}^2, \mathcal{H}^2_{A^{(0)}}(\mathbb{R}^2)) \cap \mathcal{H}_\tau.$$

As $H_{\rm per}(k)$ basically describes a Schrödinger particle in a box, it is bounded from below and has a compact resolvent for every $k \in M^*$. Hence $H_{\rm per}(k)$ has discrete spectrum with eigenvalues $E_n(k)$ of finite multiplicity that accumulate at infinity. So let

$$E_1(k) \le E_2(k) \le \cdots$$

be the eigenvalues, repeated according to their multiplicity. In the following, $k \mapsto E_n(k)$ will be called the n-th band function or just the n-th Bloch band; see Figure 1. Since $H_{\rm per}(k)$ is τ-equivariant, i.e.,

$$H_{\rm per}(k - \gamma^*) = \tau(\gamma^*) H_{\rm per}(k) \tau(\gamma^*)^{-1},$$

and $\tau(\gamma^*)$ is unitary, the Bloch bands $E_n(k)$ are Γ^*-periodic functions.

The effective Hamiltonians that we construct will be associated with isolated families of Bloch bands of the unperturbed operator $H_{\rm per}(k)$.

Definition 2.1. A family of bands $\{E_n(k)\}_{n\in I}$ with $I = [I_-, I_+] \cap \mathbb{N}$ is called isolated, or synonymously is said to satisfy the gap condition, if

$$\inf_{k\in M^*} \operatorname{dist}\big(\textstyle\bigcup_{n\in I}\{E_n(k)\}, \bigcup_{m\notin I}\{E_m(k)\}\big) =: c_{\rm g} > 0.$$

We say that $\{E_n(k)\}_{n\in I}$ is strictly isolated with strict gap $d_{\rm g}$ if, for

$$\sigma_I := \overline{\textstyle\bigcup_{n\in I} \bigcup_{k\in M^*}\{E_n(k)\}},$$

we have that

$$\inf_{m\notin I,\, k\in M^*} \operatorname{dist}(E_m(k), \sigma_I) := d_{\mathrm{g}} > 0.$$

By $P_I(k)$ we denote the spectral projection of $H_{\mathrm{per}}(k)$ corresponding to the isolated family of eigenvalues $\{E_n(k)\}_{n\in I}$. Because of the gap condition, the map

$$\mathbb{R}^2 \to \mathcal{L}(\mathcal{H}_{\mathrm{f}}), \quad k \mapsto P_I(k),$$

is real analytic and with $H_{\mathrm{per}}(k)$ also τ-equivariant. This family of projections defines a vector bundle over the torus $\mathbb{T}^* := \mathbb{R}^2/\Gamma^*$.

Definition 2.2. Let the bundle $\pi : \Xi_\tau \to \mathbb{T}^*$ with typical fiber $\mathcal{H}_{\mathrm{f}}$ be given by

$$\Xi_\tau := (\mathbb{R}^2 \times \mathcal{H}_{\mathrm{f}})/\sim_\tau,$$

where

$$(k, \varphi) \sim_\tau (k', \varphi') \qquad \Longleftrightarrow \qquad k' = k - \gamma^* \quad \text{and} \quad \varphi' = \tau(\gamma^*)\varphi \quad \text{for some } \gamma^* \in \Gamma^*.$$

The Bloch bundle Ξ_{Bl} associated to the isolated family $\{E_n(k)\}_{n\in I}$ of Bloch bands is the subbundle given by

$$\Xi_{\mathrm{Bl}} := \{(k, \varphi) \in \mathbb{R}^2 \times \mathcal{H}_{\mathrm{f}} \mid \varphi \in P(k)\mathcal{H}_{\mathrm{f}}\}/\sim_\tau. \tag{8}$$

Hence, the L^2-sections of Ξ_τ are in one-to-one correspondence with elements of $\mathcal{H}_\tau$ and the L^2-sections of the Bloch bundle are in one-to-one correspondence with functions $f \in \mathcal{H}_\tau$ that satisfy $P_I(k) f(k) = f(k)$ for all $k \in \mathbb{R}^2$.

H^ε as a pseudodifferential operator on $\mathcal{H}_\tau$. The operator of multiplication by x on $L^2(\mathbb{R}^2)$ is mapped under the Bloch–Floquet transformation to the operator $\mathrm{i}\nabla_k^\tau := \mathcal{U}_{\mathcal{F}} x \mathcal{U}_{\mathcal{F}}^*$. A simple computation shows that $\mathrm{i}\nabla_k^\tau$ acts as the gradient with domain $H^1_{\mathrm{loc}}(\mathbb{R}^2, \mathcal{H}_{\mathrm{f}}) \cap \mathcal{H}_\tau \subset \mathcal{H}_\tau$. Hence, by the functional calculus for self-adjoint operators, the full Hamiltonian H^ε takes the form

$$H^\varepsilon_{\mathrm{BF}} := \mathcal{U}_{\mathrm{BF}} H^\varepsilon \mathcal{U}^*_{\mathrm{BF}} = \tfrac{1}{2}(-\mathrm{i}\nabla_y - A^{(0)}(y) + k - A(\mathrm{i}\varepsilon\nabla_k^\tau))^2 + V_\Gamma(y) + \Phi(\mathrm{i}\varepsilon\nabla_k^\tau),$$

where we put $A := A^{(1)} + A^{(2)}$ and use that $\varepsilon A^{(1)}(x) = A^{(1)}(\varepsilon x)$ due to linearity. One key step for the following analysis is to interpret $H^\varepsilon_{\mathrm{BF}}$ as a pseudodifferential operator with operator-valued symbol

$$H(k, r) := \tfrac{1}{2}(-\mathrm{i}\nabla_y - A^{(0)}(y) + k - A(r))^2 + V_\Gamma(y) + \Phi(r) \tag{9}$$

under the quantization map $k \mapsto k$ and $r \mapsto \mathrm{i}\varepsilon\nabla_k^\tau$. To make this precise, note that $H(k, r)$ is a τ-equivariant symbol taking values in the self-adjoint operators on $\mathcal{H}_{\mathrm{f}}$ with domain $\mathcal{H}^2_{A^{(0)}}$ independent of (k, r). For the convenience of the reader we briefly give the definitions of the relevant symbol classes and refer to [Teufel 2003, Appendix B] for details on the τ-quantization.

Definition 2.3. A function $w : \mathbb{R}^4 \to [0, \infty)$ satisfying, for some $C, N > 0$,

$$w(x) \le C\langle x - y\rangle^N w(y) \quad \text{for all } x, y \in \mathbb{R}^4,$$

is called an order function. Here $\langle x\rangle := (1 + |x|^2)^{1/2}$.

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces and w an order function. Then by $S^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ we denote the space functions $f \in C^\infty(\mathbb{R}^4, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$, which satisfy

$$\|f\|_{w,\alpha,\beta} := \sup_{(k,r)\in\mathbb{R}^4} w(k,r)^{-1} \|(\partial_k^\alpha \partial_r^\beta f)(k,r)\|_{\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2)} < \infty \quad \text{for all } \alpha, \beta \in \mathbb{N}_0^2.$$

Functions in $S^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ are called operator-valued symbols with order function w. For the constant order function $w(k,r) \equiv 1$ we write $S^1(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)) := S^{w\equiv 1}(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$.

Let $\tau_j : \Gamma^* \to \mathcal{L}(\mathcal{H}_j)$, $j = 1, 2$, be unitary representations. A symbol $f \in S^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ is called (τ_1, τ_2)-equivariant if

$$f(k-\gamma^*, r) = \tau_2(\gamma^*) f(k,r) \tau_1(\gamma^*)^{-1} \quad \text{for all } \gamma^* \in \Gamma^* \text{ and } (k,r) \in \mathbb{R}^4.$$

The corresponding space is denoted by $S^w_{(\tau_1,\tau_2)}(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ and equipped with the Fréchet metric induced by the family of seminorms $\|\cdot\|_{w,\alpha,\beta}$.

We denote by $S^w_{(\tau_1,\tau_2)}(\varepsilon, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ the space of uniformly bounded functions

$$f : [0, \varepsilon_0) \to S^w_{(\tau_1,\tau_2)}(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)).$$

If $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}$ and $\tau_1 = \tau_2$, we write $S^w_\tau(\varepsilon, \mathcal{L}(\mathcal{H}))$ instead.

Proposition 2.4. *Let $w_A(k,r) := 1 + |k - A(r)|^2$. Then the operator-valued function $(k,r) \mapsto H(k,r)$ defined in* (9) *is a symbol $H \in S^{w_A}_{(\tau_1,\tau_2)}(\mathcal{L}(\mathcal{H}^2_{A(0)}, \mathcal{H}_{\mathrm{f}}))$ with $\tau_1 = \tau|_{\mathcal{H}^2_{A(0)}}$ and $\tau_2 = \tau$.*

Proof. Since $H(k,r) = H_{\mathrm{per}}(k - A(r)) + \Phi(r)$, all claims can be checked explicitly on H_{per} using Assumption 1: the (τ_1, τ_2)-equivariance of H follows from the (τ_1, τ_2)-equivariance of H_{per}, and $H_{\mathrm{per}} \in S^{w_0}_{(\tau_1,\tau_2)}(\mathcal{L}(\mathcal{H}^2_{A(0)}, \mathcal{H}_{\mathrm{f}}))$ with $w_0(k,r) := 1 + |k|^2$ implies $H \in S^{w_A}_{(\tau_1,\tau_2)}(\mathbb{R}^4, \mathcal{L}(\mathcal{H}^2_{A(0)}, \mathcal{H}_{\mathrm{f}}))$. See [De Nittis and Panati 2010, Lemma 3.8] for details on the last argument. □

Note that the Weyl quantization of a symbol f in $S^w_{(\tau_1,\tau_2)}(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ defines an operator $\mathrm{Op}^{(\tau_1,\tau_2)}(f)$ that maps $\mathcal{H}_1$-valued, τ_1-equivariant functions to $\mathcal{H}_2$-valued, τ_2-equivariant functions. For details on this τ-quantization, see [Teufel 2003, Appendix B]. For a general introduction to pseudodifferential operators with operator-valued symbols in the same context, we refer to [Gérard et al. 1991].

Since the (τ_1, τ_2)-quantization $\mathrm{Op}^{(\tau_1,\tau_2)}(H)$ of H restricted to the space of smooth τ-equivariant functions with values in $\mathcal{H}^2_{A(0)}(\mathbb{R}^2)$ agrees with the restriction of $H^\varepsilon_{\mathcal{F}}$, and since both operators are essentially self-adjoint on this subspace, their closures agree and we will identify them in the following.

3. Almost invariant subspaces

The first step of space-adiabatic perturbation theory is the construction of the almost invariant subspace $\Pi^\varepsilon_I \mathcal{H}_\tau$ associated with an isolated family of Bloch bands $\{E_n(k)\}_{n\in I}$. Here Π^ε_I is an orthogonal projection almost commuting with $H^\varepsilon_{\mathcal{F}}$. This concept goes back to [Nenciu 2002] and the general construction was introduced in [Nenciu and Sordoni 2004; Martinez and Sordoni 2002] based on techniques developed already in [Helffer and Sjöstrand 1990a]. The application to the case of nonmagnetic Bloch bands including the τ-equivariant Weyl calculus was worked out in [Panati et al. 2003a; Teufel 2003]. Since these methods carry over to the case of magnetic Bloch bands without difficulties — see also [Dimassi et al. 2004; Stiepan 2011] — we skip the details of the proof. Note, however, that we add a new observation to the statement: under the assumption of a strict gap and for sufficiently small perturbations, the resulting projection Π^ε_I actually commutes with $H^\varepsilon_{\mathrm{BF}}$, since it turns out to be a spectral projection.

Theorem 3.1. *Let Assumptions 1 and 2 hold and let $\{E_n(k)\}_{n\in I}$ be an isolated family of Bloch bands. Then there exists an orthogonal projection $\Pi^\varepsilon_I \in \mathcal{L}(\mathcal{H}_\tau)$ such that $H^\varepsilon_{\mathrm{BF}}\Pi^\varepsilon_I$ is a bounded operator and*

$$\|[H^\varepsilon_{\mathrm{BF}}, \Pi^\varepsilon_I]\| = \mathbb{O}(\varepsilon^\infty).$$

Moreover, Π^ε_I is close to a pseudodifferential operator $\mathrm{Op}^\tau(\pi)$:

$$\|\Pi^\varepsilon_I - \mathrm{Op}^\tau(\pi)\| = \mathbb{O}(\varepsilon^\infty), \tag{10}$$

where $\pi \in S^1_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_{\mathrm{f}})) := S^{w\equiv 1}_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_{\mathrm{f}}))$ with principal symbol $\pi_0(k, r) = P_I(k - A(r))$.

If $\{E_n(k)\}_{n\in I}$ is strictly isolated with gap d_{g} and $\|\Phi\|_\infty < \frac{1}{2}d_{\mathrm{g}}$, then (10) *holds for Π^ε_I being the spectral projection of $H^\varepsilon_{\mathrm{BF}}$ associated to the interval $\left[\inf E_I - \frac{1}{2}d_{\mathrm{g}}, \sup E_I + \frac{1}{2}d_{\mathrm{g}}\right]$. In particular, $[H^\varepsilon_{\mathrm{BF}}, \Pi^\varepsilon_I] = 0$ in this case.*

Proof. The construction of Π^ε_I is given in [Teufel 2003, Proposition 5.16] for general Hamiltonians with symbol $\widetilde{H} \in S^w_{(\tau_1,\tau_2)}(\mathbb{R}^4, \mathcal{L}(\mathfrak{D}, \mathcal{H}_{\mathrm{f}}))$ for $w(k, r) = 1 + |k|^2$, where $\widetilde{H}(k, r)$ is pointwise a self-adjoint operator on $\mathcal{H}_{\mathrm{f}}$ with domain $\mathfrak{D}$. In the case $A^{(1)} = 0$ it applies verbatim also to our Hamiltonian, since then $H \in S^w_{(\tau_1,\tau_2)}(\mathbb{R}^4, \mathcal{L}(\mathcal{H}^2_{A^{(0)}}, \mathcal{H}_{\mathrm{f}}))$. The slight modification that allows one to include also a linear term $A^{(1)} \neq 0$ is worked out in [De Nittis and Panati 2010, Theorem 3.12(1)], where the order function w is replaced by w_A. Note that their assumption (D) on the triviality of the Bloch bundle is not used in the proof of [De Nittis and Panati 2010, Theorem 3.12(1)]. We remark that the construction of Π^ε_I for nonzero $A^{(0)}$ and $A^{(1)} = 0$ was also done in [Stiepan 2011].

The statement for strictly isolated bands follows from inspecting, for example, the proof of [Teufel 2003, Proposition 5.16], from where the following notation is also borrowed. Under the assumption of a strict gap, the Moyal resolvent $R(\zeta)$ can be constructed globally on $\mathcal{U}_{z_0} = \mathbb{R}^4$ and for ζ in a fixed positively oriented circle $\Lambda \subset \mathbb{C}$ encircling $\left[\inf E_I - \frac{1}{2}d_{\mathrm{g}}, \sup E_I + \frac{1}{2}d_{\mathrm{g}}\right]$. But then [Teufel 2003, (5.28)] implies $\mathrm{Op}^\tau(R(\zeta)) = (\mathrm{Op}^{(\tau_1,\tau_2)}(H) - \zeta)^{-1} + \mathbb{O}(\varepsilon^\infty)$ and thus, by [ibid., (5.38)],

$$\mathrm{Op}^\tau(\pi) = \frac{\mathrm{i}}{2\pi}\oint_\Lambda \mathrm{Op}^\tau(R(\zeta))\,\mathrm{d}\zeta = \frac{\mathrm{i}}{2\pi}\oint_\Lambda (H^\varepsilon_{\mathrm{BF}} - \zeta)^{-1}\,\mathrm{d}\zeta + \mathbb{O}(\varepsilon^\infty). \qquad \square$$

4. Magnetic Bloch bundles

With respect to the (almost) invariant subspace $\Pi^\varepsilon_I\mathcal{H}_\tau$ associated to an isolated family of Bloch bands, the Hamiltonian thus takes the (almost) block diagonal form

$$H^\varepsilon_{\mathrm{BF}} = \Pi^\varepsilon_I H^\varepsilon_{\mathrm{BF}} \Pi^\varepsilon_I + (1 - \Pi^\varepsilon_I) H^\varepsilon_{\mathrm{BF}} (1 - \Pi^\varepsilon_I) + \mathbb{O}(\varepsilon^\infty),$$

where $\mathbb{O}(\varepsilon^\infty)$ holds in the operator norm. For strictly isolated bands, $\mathbb{O}(\varepsilon^\infty)$ can be replaced by zero and the prefix "almost" can be dropped. The remaining task is to show that the block $\Pi^\varepsilon_I H^\varepsilon_{\mathrm{BF}} \Pi^\varepsilon_I$ is unitarily equivalent to an effective Hamiltonian H_{eff} given by Peierls substitution on some simple reference space $\mathcal{H}_{\text{ref}}$.

Let us quickly summarize how this is achieved in the case $B_0 \equiv 0$ in [Panati et al. 2003a; Teufel 2003]. The smoothness of $H(k, r)$ and the gap condition imply the smoothness of the spectral projection $P_I(k - A(r))$. In particular, $P_I(k - A(r))$ has constant rank $m \in \mathbb{N}$. It is thus natural to choose $\mathcal{H}_{\text{ref}}$ as the $\mathbb{C}^m$-valued functions over the torus $\mathbb{T}^* = \mathbb{R}^2/\Gamma^*$, i.e., $\mathcal{H}_{\text{ref}} = L^2(\mathbb{T}^*, \mathbb{C}^m)$. As in the case of Π_I^ε, the unitary map $U^\varepsilon : \Pi_I^\varepsilon \mathcal{H}_\tau \to \mathcal{H}_{\text{ref}}$ is constructed perturbatively order by order as the quantization of a semiclassical symbol $u(k, r) \asymp \sum_{j=0}^{\infty} \varepsilon^j u_j(k, r)$. The starting point of the construction is a unitary map $u_0(k, r) : P_I(k - A(r))\mathcal{H}_{\text{f}} \to \mathbb{C}^m$ that is smooth and right-τ-equivariant:

$$u_0(k - \gamma^*, r) = u_0(k, r)\tau(\gamma^*)^{-1} \quad \text{for all } k \in \mathbb{R}^2 \text{ and } \gamma^* \in \Gamma^*.$$

In geometric terms this means that we seek a $U(m)$-bundle isomorphism between the Bloch bundle Ξ_{Bl} and the trivial bundle over the torus $\mathbb{T}^*$ with fiber $\mathbb{C}^m$. But such an isomorphism exists if and only if the Bloch bundle is trivial. It was shown in [Helffer and Sjöstrand 1989] for the case $m = 1$ and in [Panati 2007] also for $m \geq 1$ that, in the case $B_0 = 0$, time-reversal-invariance implies that the Bloch bundle associated to any isolated family of Bloch bands is indeed trivial and hence an appropriate u_0 always exists.

However, H_{MB} is no longer time-reversal-invariant when $B_0 \neq 0$ and the Bloch bundle is in general a nontrivial vector bundle over the torus. Indeed, its nonvanishing Chern numbers are closely related to the quantum Hall effect, as was first discovered in the seminal paper [Thouless et al. 1982]. The nontriviality of magnetic Bloch bundles is the main obstruction for defining Peierls substitution for magnetic Bloch bands in any straightforward way.

Let us start with a rough sketch of our strategy for overcoming this obstruction. Our reference space $\mathcal{H}_{\text{ref}} = \mathcal{H}_\alpha$ now contains sections of a nontrivial vector bundle Ξ_α over $\mathbb{T}^*$ with typical fiber $\mathbb{C}^m$ that is isomorphic to the Bloch bundle Ξ_{Bl}. According to a result of Panati [2007], Ξ_α is uniquely characterized, up to isomorphisms, by its rank $m \in \mathbb{N}$ and its Chern number $\theta \in \mathbb{Z}$. Of course we could just glue together local trivializations of Ξ_{Bl} by suitable transition functions in order to construct such a bundle Ξ_α. However, for the definition of the map $U^\varepsilon : \Pi_I^\varepsilon \mathcal{H}_\tau \to \mathcal{H}_\alpha$ and for the construction of an appropriate pseudodifferential calculus on $\mathcal{H}_\alpha$, it will be essential to have an explicit characterization of Ξ_α with certain additional properties. To this end, we first explicitly define a global trivialization of the extended Bloch bundle given by

$$\Xi'_{\text{Bl}} := \{(k, \varphi) \in \mathbb{R}^2 \times \mathcal{H}_{\text{f}} \mid \varphi \in P_I(k)\mathcal{H}_{\text{f}}\} \tag{11}$$

over the contractible base space $\mathbb{R}^2$, i.e., an orthonormal basis $(\varphi_1(k), \dots, \varphi_m(k))$ of $P(k)\mathcal{H}_{\text{f}}$ depending smoothly on $k \in \mathbb{R}^2$. For this we use the parallel transport with respect to the Berry connection $\nabla_k^{\text{B}} = P_I(k)\nabla_k P_I(k) + P_I^\perp(k)\nabla_k P_I^\perp(k)$. Then $\Xi_\alpha := (\mathbb{R}^2 \times \mathbb{C}^m)/\sim_\alpha$ is defined in terms of the "transition function" $\alpha : \mathbb{R}^2/\Gamma^* \times \Gamma^* \to \mathcal{L}(\mathbb{C}^m)$ defined by $\varphi(k - \gamma^*) =: \alpha(k, \gamma^*)\tau(\gamma^*)\varphi(k)$. But the functions $\varphi_j(k)$ are not τ-equivariant and their derivatives of order n grow like $|k|^n$. Thus they cannot be used directly to define a symbol of the form $u_0(k, r)_{ij} = |e_i\rangle\langle\varphi_j(k - A(r))|$. However, they do give the starting point for the perturbative construction of a unitary $U_1^\varepsilon : \Pi_I^\varepsilon \mathcal{H}_\tau \to P_I \mathcal{H}_\tau$ by setting $u_0(k, r)_{ij} := |\varphi_i(k)\rangle\langle\varphi_j(k - A(r))|$, which is a good τ-equivariant symbol. From the frame $(\varphi_1(k), \dots, \varphi_m(k))$ we also get a bundle isomorphism between Ξ_{Bl} and Ξ_α, that is, a unitary map

$$U_\alpha : P_I \mathcal{H}_\tau \to \mathcal{H}_\alpha, \quad \varphi(k) \mapsto (U_\alpha \varphi)_j(k) := \langle \varphi_j(k), \varphi(k) \rangle_{\mathcal{H}_\mathrm{f}},$$

where $P_I \mathcal{H}_\tau = \{ f \in \mathcal{H}_\tau \mid f(k) = P_I(k) f(k) \}$ contains the L^2-sections of the Bloch bundle. But U_α is not a pseudodifferential operator and thus it is not clear a priori if

$$H_{\mathrm{eff}} := U_\alpha U_1^\varepsilon \Pi_I^\varepsilon \operatorname{Op}^\tau(H) \Pi_I^\varepsilon U_1^{\varepsilon *} U_\alpha^*$$

is a pseudodifferential operator and how its principal symbol looks. This problem will be solved by introducing a Weyl quantization adapted to the geometry of the Bloch bundle, for which the action of U_α is explicit.

After this rough sketch of the general strategy, let us start with the construction of the frame $(\varphi_1(k), \dots, \varphi_m(k))$. For this we need a lemma on the properties of the Berry connection.

Lemma 4.1. *On the trivial bundle $\mathbb{R}^2 \times \mathcal{H}_\mathrm{f}$ the Berry connection*

$$\nabla_k^{\mathrm{B}} := P_I(k) \nabla_k P_I(k) + P_I^\perp(k) \nabla_k P_I^\perp(k)$$

is a metric connection.

For arbitrary $x, y \in \mathbb{R}^2$ let $t^{\mathrm{B}}(x, y)$ be the parallel transport with respect to the Berry connection along the straight line from y to x. Then $t^{\mathrm{B}}(x, y) \in \mathcal{L}(\mathcal{H}_\mathrm{f})$ is unitary, satisfies

$$t^{\mathrm{B}}(x, y) = P_I(x) t^{\mathrm{B}}(x, y) P_I(y) + P_I^\perp(x) t^{\mathrm{B}}(x, y) P_I^\perp(y) \tag{12}$$

and is τ-equivariant:

$$t^{\mathrm{B}}(x - \gamma^*, y - \gamma^*) = \tau(\gamma^*) t^{\mathrm{B}}(x, y) \tau(\gamma^*)^{-1}. \tag{13}$$

Proof. Let $\psi, \phi : \mathbb{R}^2 \to \mathcal{H}_\mathrm{f}$ be smooth functions; then a simple computation yields

$$\nabla \langle \psi(k), \phi(k) \rangle_{\mathcal{H}_\mathrm{f}} = \langle \nabla^{\mathrm{B}} \psi(k), \phi(k) \rangle_{\mathcal{H}_\mathrm{f}} + \langle \psi(k), \nabla^{\mathrm{B}} \phi(k) \rangle_{\mathcal{H}_\mathrm{f}},$$

showing that ∇^{B} is metric. As a consequence, $t^{\mathrm{B}}(x, y) \in \mathcal{L}(\mathcal{H}_\mathrm{f})$ is unitary. Let $x(s) := y + s(x - y)$, $s \in [0, 1]$, be the straight line from y to x. Then $t^{\mathrm{B}}(x(s), y) =: t^B(s)$ is the unique solution of

$$\frac{\mathrm{d}}{\mathrm{d}s} t^B(s) = [(x - y) \cdot \nabla P_I(x(s)), P_I(x(s))] t^B(s) \quad \text{with} \quad t^B(0) = \mathbf{1}_{\mathcal{H}_\mathrm{f}}. \tag{14}$$

From this and $\nabla P_I = P_I (\nabla P_I) P_I^\perp + P_I^\perp (\nabla P_I) P_I$, one easily computes that

$$\frac{\mathrm{d}}{\mathrm{d}s} \big(t^B(s)^* P_I(x(s)) t^B(s) \big) = 0,$$

which implies $t^B(s)^* P_I(x(s)) t^B(s) = P_I(y)$ for all $s \in [0, 1]$, and thus (12). Now $t^B(x(s) - \gamma^*, y - \gamma^*) := \tilde{t}^B(s)$ is the unique solution of

$$\frac{\mathrm{d}}{\mathrm{d}s} \tilde{t}^B(s) = [(x - y) \cdot \nabla P_I(x(s) - \gamma^*), P_I(x(s) - \gamma^*)] \tilde{t}^B(s) \quad \text{with} \quad \tilde{t}^B(0) = \mathbf{1}_{\mathcal{H}_\mathrm{f}}. \tag{15}$$

Thus, the τ-equivariance of $t^{\mathrm{B}}(x, y)$ follows from comparing (14) and (15) and using the τ-equivariance of the projection $P_I(k)$. □

Proposition 4.2. *Let $\{E_n(k)\}_{n\in I}$ be an isolated family of Bloch bands with $|I| = m$. There are functions $\varphi_j \in C^\infty(\mathbb{R}^2, \mathcal{H}_\mathrm{f})$, $j = 1, \ldots, m$, such that $(\varphi_1(k), \ldots, \varphi_m(k))$ is an orthonormal basis of $P_I(k)\mathcal{H}_\mathrm{f}$ for all $k \in \mathbb{R}^2$ and having the following property: there is a function $\alpha : \mathbb{R}/\mathbb{Z} \to \mathcal{L}(\mathbb{C}^m)$ taking values in the unitary matrices such that*

$$\varphi(k - \gamma^*) = \alpha(\kappa_2)^{n_1} \tau(\gamma^*)\varphi(k)$$

for all $\gamma^* =: n_1\gamma_1^* + n_2\gamma_2^* \in \Gamma^*$, $k \in \mathbb{R}^2$ and $\kappa_2 := \langle k, \gamma_2\rangle/(2\pi)$. If the rank m of the Bloch bundle is 1, *then $\varphi = \varphi_1$ can be chosen so that*

$$\alpha(\kappa_2) = \mathrm{e}^{-\mathrm{i}2\pi\theta\kappa_2} = \mathrm{e}^{-\mathrm{i}\theta\langle k,\gamma_2\rangle}, \tag{16}$$

where $\theta \in \mathbb{Z}$ is the Chern number of the Bloch bundle.

Proof. Note that if the Bloch bundle is trivial then any trivializing frame $(\varphi_j(k))_{j=1,\ldots,m}$ would do the job and $\alpha \equiv \mathbf{1}_{m\times m}$. In general, we construct a trivializing frame of the extended Bloch bundle Ξ'_{Bl} (see (11)) by using the parallel transport with respect to the Berry connection.

Throughout this proof, we use instead of cartesian coordinates the coordinates $\kappa_j := \langle k, \gamma_j\rangle/(2\pi)$, namely $k = \kappa_1\gamma_1^* + \kappa_2\gamma_2^*$. In particular, we also identify $\gamma^* = (n_1, n_2) \in \Gamma^*$ with $(n_1, n_2) \in \mathbb{Z}^2$.

Let $\kappa_2 \mapsto (h_1(\kappa_2), \ldots, h_m(\kappa_2))$ be a smooth, τ_2-equivariant, orthonormal frame of $\Xi'_{\mathrm{Bl}}|_{\kappa_1=0}$, i.e., $h_j(\kappa_2 - n_2) = \tau((0, n_2))h_j(\kappa_2)$ and $(h_1(\kappa_2), \ldots, h_m(\kappa_2))$ is an orthonormal basis of $P_I((0, \kappa_2))\mathcal{H}_\mathrm{f}$. Since every complex vector bundle over the circle is trivial, such a frame always exists. Now we define a global frame of E'_{Bl} by parallel transport of h along the γ_1^*-direction,

$$\tilde{\varphi}_j(\kappa_1, \kappa_2) := t^{\mathrm{B}}((\kappa_1, \kappa_2), (0, \kappa_2))h_j(\kappa_2).$$

By Lemma 4.1, the functions $\tilde{\varphi}_j : \mathbb{R}^2 \to \mathcal{H}_\mathrm{f}$ are smooth and $(\tilde{\varphi}_1(k), \ldots, \tilde{\varphi}_m(k))$ is an orthonormal basis of $P_I(k)\mathcal{H}_\mathrm{f}$ for all $k \in \mathbb{R}^2$. Since $\tau(\gamma^*) : \operatorname{ran} P_I(k) \to \operatorname{ran} P_I(k + \gamma^*)$ is unitary for all $k \in \mathbb{R}^2$, we have that

$$\tilde{\varphi}_j(k - \gamma^*) =: \sum_{i=1}^{m} \tilde{\alpha}_{ji}(k, \gamma^*)\tau(\gamma^*)\tilde{\varphi}_i(k) \tag{17}$$

with a unitary $m \times m$ matrix $\tilde{\alpha}(k, \gamma^*) = (\tilde{\alpha}_{ji}(k, \gamma^*))_{j,i=1,\ldots,m}$. The τ-equivariance of h implies

$$\tilde{\alpha}((0, \kappa_2), (0, n_2)) = \mathbf{1}_{m\times m} \quad \text{for all } \kappa_2 \in \mathbb{R} \text{ and } n_2 \in \mathbb{Z}.$$

From the τ-equivariance (13) of the parallel transport, this also implies

$$\tilde{\alpha}(k, (0, n_2)) = \mathbf{1}_{m\times m} \quad \text{for all } k \in \mathbb{R}^2 \text{ and } n_2 \in \mathbb{Z}, \tag{18}$$

since

$$t^{\mathrm{B}}((\kappa_1, \kappa_2 - n_2), (0, \kappa_2 - n_2))\tau((0, n_2))t^{\mathrm{B}}((0, \kappa_2), (\kappa_1, \kappa_2)) \\ = \tau((0, n_2))t^{\mathrm{B}}((\kappa_1, \kappa_2), (0, \kappa_2))\tau((0, n_2))^{-1}\tau((0, n_2))t^{\mathrm{B}}((0, \kappa_2), (\kappa_1, \kappa_2)) = \tau((0, n_2)).$$

From the definition (17) it follows that $\tilde{\alpha}$ satisfies the cocycle condition

$$\tilde{\alpha}(k - \tilde{\gamma}^*, \gamma^*)\tilde{\alpha}(k, \tilde{\gamma}^*) = \tilde{\alpha}(k, \gamma^* + \tilde{\gamma}^*) \quad \text{for all } k \in \mathbb{R}^2 \text{ and } \gamma^*, \tilde{\gamma}^* \in \Gamma^*, \tag{19}$$

which, for $\gamma^* = (0, n_2)$ and $\tilde{\gamma}^* = (n_1, 0)$, together with (18) implies

$$\tilde{\alpha}(k, (n_1, 0)) = \tilde{\alpha}(k, (n_1, n_2)) \quad \text{for all } k \in \mathbb{R}^2 \text{ and } n_1, n_2 \in \mathbb{Z}.$$

Hence, $\tilde{\alpha}$ does not depend on n_2 and we write $\tilde{\alpha}(k, n_1)$ in the following. But then the cocycle condition (19) with $\gamma^* = (n_1, 0)$ and $\tilde{\gamma}^* = (0, n_2)$ implies

$$\tilde{\alpha}((\kappa_1, \kappa_2 - n_2), n_1)\tilde{\alpha}((\kappa_1, \kappa_2), 0) = \tilde{\alpha}((\kappa_1, \kappa_2), n_1),$$

and thus the periodicity of $\tilde{\alpha}$ as a function of κ_2.

Next we introduce the $m \times m$-matrix-valued connection coefficients of the Berry connection as

$$\begin{pmatrix} \tilde{\mathscr{A}}^1_{ji}(k) \\ \tilde{\mathscr{A}}^2_{ji}(k) \end{pmatrix} := -\frac{\mathrm{i}}{2\pi} \begin{pmatrix} \langle \tilde{\varphi}_i(k), \partial_{\kappa_1} \tilde{\varphi}_j(k)\rangle_{\mathscr{H}_\mathrm{f}} \\ \langle \tilde{\varphi}_i(k), \partial_{\kappa_2} \tilde{\varphi}_j(k)\rangle_{\mathscr{H}_\mathrm{f}} \end{pmatrix} = \begin{pmatrix} 0 \\ \tilde{\mathscr{A}}^2_{ji}(k) \end{pmatrix},$$

where $\tilde{\mathscr{A}}^1_{ji}(k) = 0$ because the $\tilde{\varphi}_i$ are parallel along the γ_1^*-direction. From (18) we infer that $\tilde{\mathscr{A}}^2$ is periodic in the γ_2^*-direction, that is, that $\tilde{\mathscr{A}}^2(\kappa_1, \kappa_2 + n_2) = \tilde{\mathscr{A}}^2(\kappa_1, \kappa_2)$ for all $k \in \mathbb{R}^2$ and $n_2 \in \mathbb{Z}$.

If we differentiate both sides of (17) with respect to κ_ℓ and then project on $\tilde{\varphi}_s(k - \gamma^*)$, we obtain

$$\begin{aligned} 2\pi \mathrm{i} \tilde{\mathscr{A}}^\ell_{js}(k - \gamma^*) &= \sum_{i=1}^m \bigl(\langle \tilde{\varphi}_s(k - \gamma^*), \partial_{\kappa_\ell} \tilde{\alpha}_{ji}(k, n_1) \tau(\gamma^*) \tilde{\varphi}_i(k) + \tilde{\alpha}_{ji}(k, n_1) \tau(\gamma^*) \partial_{\kappa_\ell} \tilde{\varphi}_i(k) \rangle \bigr) \\ &= \sum_{i=1}^m \partial_{\kappa_\ell} \tilde{\alpha}_{ji}(k, n_1) \overline{\tilde{\alpha}_{si}(k, n_1)} + 2\pi \mathrm{i} \sum_{i,n=1}^m \tilde{\alpha}_{ji}(k, n_1) \tilde{\mathscr{A}}^\ell_{in}(k) \overline{\tilde{\alpha}_{sn}(k, n_1)}. \end{aligned}$$

Since $\tilde{\mathscr{A}}^1_{ji}(k) = 0$, the matrix $\tilde{\alpha}(k, n_1)$ is independent of κ_1 and satisfies the linear, first-order ODE

$$\partial_{\kappa_2} \tilde{\alpha}(\kappa_2, n_1) = 2\pi \mathrm{i} (\tilde{\mathscr{A}}^2(0, \kappa_2) \tilde{\alpha}(\kappa_2, n_1) - \tilde{\alpha}(\kappa_2, n_1) \tilde{\mathscr{A}}^2(n_1, \kappa_2)). \tag{20}$$

Since $\tilde{\alpha}(\kappa_2, \cdot) : \mathbb{Z} \to \mathscr{L}(\mathbb{C}^m)$ is a group homomorphism for every $\kappa_2 \in \mathbb{R}/\mathbb{Z}$, we can put $\tilde{\alpha}(\kappa_2, n_1) = \alpha(\kappa_2)^{n_1}$ with $\alpha(\kappa_2) := \tilde{\alpha}(\kappa_2, 1)$. This proves the statement of the lemma for the case $m > 1$ by setting $\varphi := \tilde{\varphi}$.

For $m = 1$ we evaluate the solution of (20) in order to obtain an explicit expression for α,

$$\tilde{\alpha}(\kappa_2, 1) = \exp\biggl(2\pi \mathrm{i} \int_0^{\kappa_2} \mathrm{d}s \, (\tilde{\mathscr{A}}^2(0, s) - \tilde{\mathscr{A}}^2(1, s)) \biggr).$$

Introducing the curvature of the Berry connection,

$$\Omega(k) = \frac{|M^*|}{2\pi} \partial_{\kappa_1} \tilde{\mathscr{A}}^2(k),$$

by Stokes' theorem we have

$$2\pi \int_0^{\kappa_2} (\tilde{\mathscr{A}}^2(1, s) - \tilde{\mathscr{A}}^2(0, s)) \, \mathrm{d}s = \frac{4\pi^2}{|M^*|} \int_0^{\kappa_2} \int_0^1 \Omega(p, s) \, \mathrm{d}p \, \mathrm{d}s =: \overline{\Omega}(\kappa_2)$$

and thus

$$\tilde{\alpha}(\kappa_2, 1) = \mathrm{e}^{-\mathrm{i}\overline{\Omega}(\kappa_2)}.$$

To obtain the simpler form claimed in the lemma, we put

$$\varphi(k) := \mathrm{e}^{\mathrm{i}\kappa_1(2\pi\kappa_2\theta - \overline{\Omega}(\kappa_2))}\tilde{\varphi}(k),$$

where $\theta := \overline{\Omega}(1)/(2\pi)$ is the Chern number of the Bloch bundle. Hence,

$$\varphi(k-\gamma^*) = \mathrm{e}^{-\mathrm{i}2\pi\theta\kappa_2 n_1}\tau(\gamma^*)\varphi(k). \qquad \square$$

Proposition 4.3. *Let Assumptions 1 and 2 hold with $A^{(1)} = 0$ and let $\{E_n(k)\}_{n\in I}$ be an isolated family of Bloch bands. Then there exists a unitary operator $U_1^\varepsilon \in \mathcal{L}(\mathcal{H}_\tau)$ such that*

$$U_1^\varepsilon \Pi_I^\varepsilon U_1^{\varepsilon *} = P_I$$

and $U_1^\varepsilon = \mathrm{Op}^\tau(u) + \mathbb{O}_0(\varepsilon^\infty)$, where $u \asymp \sum_{j\geq 0}\varepsilon^j u_j$ belongs to $S_\tau^1(\varepsilon, \mathcal{L}(\mathcal{H}_\mathrm{f}))$ and has the τ-equivariant principal symbol $u_0(k,r) = \sum_{i=1}^m |\varphi_i(k)\rangle\langle\varphi_i(k-A(r))| + u_0^\perp(k,r)$.

Proof. We only need to show that a τ-equivariant principal symbol $u_0(k,r)$ of the form claimed above exists. Then the proof works line by line as the proof of [Teufel 2003, Proposition 5.18]; see also [Panati et al. 2003a]. However, according to Lemma 4.1,

$$u_0(k,r) := t^\mathrm{B}(k, k-A(r)) = t^\mathrm{B}((\kappa_1,\kappa_2),(\kappa_1 - A_1(r),\kappa_2))$$

is τ-equivariant and has the desired form. Here we use the choice of gauge $\gamma_2 \cdot A(r) = 0$ and write as before $A(r) = A_1(r)\gamma_1^*$. Note that at this point we have to assume $A^{(1)} \equiv 0$, because otherwise the κ_2-derivatives of u_0 would become unbounded functions of r and $u_0 \notin S_\tau^w$ for all order functions w. $\square$

Definition 4.4. Using the matrix-valued function α constructed in Proposition 4.2, we define

$$\mathcal{H}_\alpha := \{f \in L^2_{\mathrm{loc}}(\mathbb{R}^2, \mathbb{C}^m) \mid f(k-\gamma^*) = \alpha(\kappa_2)^{-n_1} f(k) \;\text{ for all }\; k \in \mathbb{R}^2,\ \gamma^* \in \Gamma^*\}$$

with inner product $\langle f, g\rangle_{\mathcal{H}_\alpha} = \int_{M^*} \mathrm{d}k\, \langle f(k), g(k)\rangle_{\mathbb{C}^m}$.

Using the orthonormal frame $(\varphi_1(k), \dots, \varphi_m(k))$ constructed in Proposition 4.2, we define the unitary maps

$$U_\alpha(k) : P_I(k)\mathcal{H}_\mathrm{f} \to \mathbb{C}^m, \quad f \mapsto (U_\alpha(k) f)_i := \langle \varphi_i(k), f\rangle_{\mathcal{H}_\mathrm{f}},$$
$$U_\alpha : P_I\mathcal{H}_\tau \to \mathcal{H}_\alpha, \qquad f \mapsto (U_\alpha f)(k)_i := \langle \varphi_i(k), f(k)\rangle_{\mathcal{H}_\mathrm{f}}.$$

In the same way that $P_I\mathcal{H}_\tau$ is the space of L^2-sections of the Bloch bundle Ξ_{Bl}, the space $\mathcal{H}_\alpha$ is the space of L^2-sections of a bundle Ξ_α.

Definition 4.5. Let

$$\Xi_\alpha := (\mathbb{R}^2 \times \mathbb{C}^m)/\sim_\alpha, \tag{21}$$

where

$$(k,\lambda) \sim_\alpha (k',\lambda') \quad\iff\quad k' = k - \gamma^* \;\text{ and }\; \lambda' = \alpha(\kappa_2)^{-n_1}\lambda \;\text{ for some }\; \gamma^* = (n_1, n_2) \in \Gamma^*.$$

On sections of Ξ_α we define the connection $\nabla^\alpha := U_\alpha \nabla^\mathrm{B} U_\alpha^*$.

It was shown by Panati [2007] that even for $m > 1$ the bundle Ξ_α is, up to isomorphisms, uniquely determined by its Chern number

$$\theta := \frac{1}{2\pi}\int_{M^*} \operatorname{tr}(\Omega(k))\,\mathrm{d}k.$$

However, we use a canonical form for α only in the case $m = 1$, where a canonical choice is (16).

5. The effective Hamiltonian as a pseudodifferential operator

Combining the unitary maps $U_1^\varepsilon : \Pi_I^\varepsilon \mathcal{H}_\tau \to P_I \mathcal{H}_\tau$ and $U_\alpha : P_I \mathcal{H}_\tau \to \mathcal{H}_\alpha$ into

$$U^\varepsilon : \Pi_I^\varepsilon \mathcal{H}_\tau \to \mathcal{H}_\alpha, \quad U^\varepsilon := U_\alpha U_1^\varepsilon,$$

we find that the block $\Pi_I^\varepsilon H_{\mathrm{BF}}^\varepsilon \Pi_I^\varepsilon$ of $H_{\mathrm{BF}}^\varepsilon$ is unitarily equivalent to the effective Hamiltonian

$$H_I^{\mathrm{eff}} := U^\varepsilon \Pi_I^\varepsilon H_{\mathrm{BF}}^\varepsilon \Pi_I^\varepsilon U^{\varepsilon *}$$

acting on the space $\mathcal{H}_\alpha$ of L^2-sections of Ξ_α. The remaining problem is to compute explicitly an asymptotic expansion of H_I^{eff} in powers of ε, where the leading-order term should be given by Peierls substitution,

$$H_I^{\mathrm{eff}} = E_I(k - A(\mathrm{i}\varepsilon\nabla_k^\alpha)) + \Phi(\mathrm{i}\varepsilon\nabla_k^\alpha) + \mathbb{O}(\varepsilon)$$

with

$$E_I(k)_{ij} = \langle \varphi_i(k), H_{\mathrm{per}}(k)\varphi_j(k)\rangle.$$

Note that ∇^α is the only natural connection on sections of Ξ_α, as the flat connection, used implicitly for Peierls substitution in the nonmagnetic case, is not at our disposal. It will be a considerable effort in itself to properly define the pseudodifferential operator $E_I(k - A(\mathrm{i}\varepsilon\nabla_k^\alpha)) + \Phi(\mathrm{i}\varepsilon\nabla_k^\alpha)$ as an operator on $\mathcal{H}_\alpha$.

In the nonmagnetic case the problem of expanding H_{eff} is much simpler. Then not only the Hamiltonian $H_{\mathrm{BF}}^\varepsilon = \mathrm{Op}^\tau(H)$ and the projection $\Pi_I^\varepsilon = \mathrm{Op}^\tau(\pi) + \mathbb{O}(\varepsilon^\infty)$ are $\mathbb{O}(\varepsilon^\infty)$-close to pseudodifferential operators, but also the intertwining unitary $U^\varepsilon = \mathrm{Op}^\tau(u) + \mathbb{O}(\varepsilon^\infty)$. Moreover, $\mathcal{H}_\alpha$ contains periodic functions and H_I^{eff} is close to a semiclassical pseudodifferential operator $h_I^{\mathrm{eff}}(k, \mathrm{i}\varepsilon\nabla_k)$ with an asymptotic expansion of its symbol computable using the Moyal product:

$$\begin{aligned} H_I^{\mathrm{eff}} = U^\varepsilon \Pi_I^\varepsilon H_{\mathrm{BF}}^\varepsilon \Pi_I^\varepsilon U^{\varepsilon *} &= \mathrm{Op}^\tau(u)\,\mathrm{Op}^\tau(\pi)\,\mathrm{Op}^\tau(H)\,\mathrm{Op}^\tau(\pi)\,\mathrm{Op}^\tau(u^*) + \mathbb{O}(\varepsilon^\infty) \\ &= \mathrm{Op}^\tau(\underbrace{u \sharp \pi \sharp H \sharp \pi \sharp u^*}_{=:h_I^{\mathrm{eff}}}) + \mathbb{O}(\varepsilon^\infty). \end{aligned}$$

In our magnetic case, however, we cannot proceed like this. Although the operators Π_I^ε and U_1^ε are again nearly pseudodifferential operators, this is no longer true for U_α. The symbol for this operator would have to be $u_\alpha(k, r) = \sum_{i=1}^m \langle \varphi_i(k)|$, which is in no suitable symbol class because its derivatives of order n grow like $|k|^n$. So we have to deal with the fact that our effective Hamiltonian is of the form

$$H_I^{\mathrm{eff}} = U^\varepsilon \Pi_I^\varepsilon\,\mathrm{Op}^\tau(H)\Pi_I^\varepsilon U^{\varepsilon *} = U_\alpha P_I\,\mathrm{Op}^\tau(\mathfrak{h}) P_I U_\alpha^* + \mathbb{O}(\varepsilon^\infty).$$

Our solution is to replace the τ-quantized operator $\mathrm{Op}^\tau(\mathfrak{h}) = \mathfrak{h}(k, \mathrm{i}\varepsilon\nabla_k^\tau)$ by a "Berry quantized" operator $\mathrm{Op}^{\mathrm{B}}(h) = h(k, \mathrm{i}\varepsilon\nabla_k^{\mathrm{B}})$ (see (26)) with a modified symbol h. Because of the unitary equivalence $\nabla^\alpha = U_\alpha \nabla^{\mathrm{B}} U_\alpha^*$, one expects and we will show that $U_\alpha h(k, \mathrm{i}\varepsilon\nabla_k^{\mathrm{B}}) U_\alpha^* = h_I^{\mathrm{eff}}(k, \mathrm{i}\varepsilon\nabla_k^\alpha)$ with $h_I^{\mathrm{eff}}(k, r)_{ij} := \langle \varphi_i(k), h(k, r)\varphi_j(k)\rangle$. We postpone the detailed definitions of the new quantizations and the proofs of their relevant properties to Section 6. In a nutshell the quantization maps are defined as follows:

- For $h \in S_\tau^1(\varepsilon, \mathcal{L}(\mathcal{H}_{\mathrm{f}}))$ we put $\mathrm{Op}^{\mathrm{B}}(h) = h(k, \mathrm{i}\varepsilon\nabla_k^{\mathrm{B}})$ acting on $\mathcal{H}_\tau$.
- For $h \in S_\alpha(\varepsilon, \mathcal{L}(\mathbb{C}^m))$ (see Definition 6.11) we put $\mathrm{Op}^\alpha(h) = h(k, \mathrm{i}\varepsilon\nabla_k^\alpha)$ acting on $\mathcal{H}_\alpha$.
- For $m = 1$ and Γ^*-periodic $h \in S^1(\varepsilon, \mathcal{L}(\mathbb{C}))$ we put $\mathrm{Op}^\theta(h) = h(k, \mathrm{i}\varepsilon\nabla_k^\theta)$ acting on $\mathcal{H}_\alpha$, where $\nabla_k^\theta := \nabla_k + \mathrm{i}\theta/(2\pi)\,\langle k, \gamma_1\rangle\gamma_2$.

The last quantization will only be used for the case $m = 1$ in order to obtain an explicit expression for H_I^{eff}. Note that changing the connection from ∇^α to ∇^θ makes the quantization rule independent of φ_1. Moreover, ∇^θ is canonical in the sense that its curvature tensor $R^\theta(X, Y) = \mathrm{i}\theta|M|/(2\pi)\,(X_1Y_2 - X_2Y_1)$ is constant.

All in all, the steps leading to a representation of the effective Hamiltonian H_I^{eff} as a pseudodifferential operator are

$$\begin{aligned} H_I^{\mathrm{eff}} &:= U^\varepsilon \Pi_I^\varepsilon H_{\mathrm{BF}}^\varepsilon \Pi_I^\varepsilon U^{\varepsilon *} = U^\varepsilon \Pi_I^\varepsilon \,\mathrm{Op}^\tau(H)\, \Pi_I^\varepsilon U^{\varepsilon *} = U_\alpha P_I\, \mathrm{Op}^\tau(\mathfrak{h}) P_I U_\alpha^* + \mathcal{O}(\varepsilon^\infty) \\ &= U_\alpha P_I\, \mathrm{Op}^B(h) P_I U_\alpha^* + \mathcal{O}(\varepsilon^\infty) = \mathrm{Op}^\alpha(h_I^{\mathrm{eff}}) + \mathcal{O}(\varepsilon^\infty). \end{aligned}$$

In the following theorem we collect our main results:

Theorem 5.1. *Let Assumptions 1 and 2 hold with $A^{(1)} = 0$ and let $\{E_n(k)\}_{n\in I}$ be an isolated family of Bloch bands. Then there exist an orthogonal projection $\Pi_I^\varepsilon \in \mathcal{L}(\mathcal{H}_\tau)$ and a unitary map $U^\varepsilon \in \mathcal{L}(\Pi_I^\varepsilon\mathcal{H}_\tau, \mathcal{H}_\alpha)$ such that*

$$\|[H_{\mathrm{BF}}^\varepsilon, \Pi_I^\varepsilon]\|_{\mathcal{L}(\mathcal{H}_\tau)} = \mathcal{O}(\varepsilon^\infty) \tag{22}$$

and, with $H_I^{\mathrm{eff}} := U^\varepsilon \Pi_I^\varepsilon H_{\mathrm{BF}}^\varepsilon \Pi_I^\varepsilon U^{\varepsilon *}$,

$$\|(\mathrm{e}^{-\mathrm{i}H_{\mathrm{BF}}^\varepsilon t} - U^{\varepsilon *}\mathrm{e}^{-\mathrm{i}H_I^{\mathrm{eff}} t} U^\varepsilon)\Pi_I^\varepsilon\|_{\mathcal{L}(\mathcal{H}_\tau)} = \mathcal{O}(\varepsilon^\infty |t|). \tag{23}$$

If $\{E_n(k)\}_{n\in I}$ is strictly isolated with gap d_{g} and $\|\Phi\|_\infty < \frac{1}{2}d_{\mathrm{g}}$, then the expressions in (22) *and* (23) *vanish exactly.*

There is an α-equivariant symbol $h_I^{\mathrm{eff}} \in S_\alpha(\varepsilon, \mathcal{L}(\mathbb{C}^m))$ such that

$$\|H_I^{\mathrm{eff}} - \mathrm{Op}^\alpha(h_I^{\mathrm{eff}})\|_{\mathcal{L}(\mathcal{H}_\alpha)} = \mathcal{O}(\varepsilon^\infty). \tag{24}$$

The asymptotic expansion of the symbol h_I^{eff} can be computed, in principle, to any order in ε. Its principal symbol is given by

$$h_0(k, r) = E_I(k - A(r)) + \Phi(r)\mathbf{1}_{m\times m},$$

where

$$E_I(k)_{ij} := \langle \varphi_i(k), H_{\mathrm{per}}(k)\varphi_j(k)\rangle_{\mathcal{H}_{\mathrm{f}}}$$

and $(\varphi_1(k),\dots,\varphi_m(k))$ *is the orthonormal frame of the extended Bloch bundle constructed in Proposition 4.2. Thus, Peierls substitution is the leading-order approximation to the restriction of the Hamiltonian to an isolated family of bands*:

$$\|H_I^{\text{eff}} - \operatorname{Op}^\alpha(h_0)\|_{\mathcal{L}(\mathcal{H}_\alpha)} = \mathcal{O}(\varepsilon).$$

Proof. The projection Π_I^ε was constructed in Theorem 3.1. The unitary $U^\varepsilon := U_\alpha U_1^\varepsilon$ is obtained from U_1^ε, constructed in Proposition 4.3, and U_α, given in Definition 4.4. Statement (23) follows from (22) by standard time-dependent perturbation theory.

Now the operator $H_0 := U_1^\varepsilon \Pi_I^\varepsilon H_{\text{BF}}^\varepsilon \Pi_I^\varepsilon U_1^{\varepsilon *}$ is, by construction, asymptotic to the τ-quantization of the semiclassical symbol $\mathfrak{h} := u \sharp \pi \sharp H \sharp \pi \sharp u^* \in S_\tau^1(\varepsilon)$ with principal symbol

$$\mathfrak{h}_0(k,r) = \big\langle \varphi_i(k - A(r)), (H_{\text{per}}(k - A(r)) + \Phi(r))\varphi_j(k - A(r))\big\rangle_{\mathcal{H}_{\text{f}}} |\varphi_i(k)\rangle\langle\varphi_j(k)|.$$

As sketched before and as to be shown in Corollary 6.9, one can approximate $\operatorname{Op}^\tau(\mathfrak{h})$ by the Berry quantization $\operatorname{Op}^{\text{B}}(h)$ of a modified symbol h up to an error of order ε^∞. More precisely, in Corollary 6.9 we show that there is a sequence of symbols $h_n \in S_\tau^1$ with $h_0 = \mathfrak{h}_0$ such that, for any $N \in \mathbb{N}$,

$$\left\| \sum_{n=0}^{N} \varepsilon^n \operatorname{Op}^{\text{B}}(h_n) - \operatorname{Op}^\tau(\mathfrak{h}) \right\| = \mathcal{O}(\varepsilon^{N+1}).$$

As we will show in Proposition 6.13, the Berry quantization transforms in an explicit way under the unitary mapping U_α to the reference space $\mathcal{H}_\alpha$. Namely, it holds that $U_\alpha \operatorname{Op}^{\text{B}}(h_n) U_\alpha^* = \operatorname{Op}^\alpha(h_n^{\text{eff}})$ with

$$(h_n^{\text{eff}})_{ij}(k,r) = \langle \varphi_i(k), h_n(k,r)\varphi_j(k)\rangle.$$

Then (24) holds for any resummation h_I^{eff} of the asymptotic series $\sum \varepsilon^n h_n^{\text{eff}}$. □

As stated in the theorem, one can compute order by order the asymptotic expansion of h_I^{eff} using the explicit expansions of the symbols π and u and expanding Moyal products. We now show how to compute the subprincipal symbol h_1 in a special case, and for this we adopt the notation introduced in the proof of Theorem 5.1. According to Corollary 6.9 there are two contributions to h_1, namely

$$h_1(k,r) = h_{1,\text{c}} + \mathfrak{h}_1 := -\tfrac{1}{2}\mathrm{i}\big(\nabla_r \mathfrak{h}_0(k,r)\cdot M(k) + M(k)\cdot \nabla_r \mathfrak{h}_0(k,r)\big) + \mathfrak{h}_1,$$

where

$$M(k) := [\nabla P_I(k), P_I(k)].$$

While one could compute h_1 also for general isolated families of bands, this is more cumbersome and the result is rather complicated. We therefore specialize to the case $m = 1$, i.e., to a single nondegenerate isolated band E_n. Then

$$\mathfrak{h}_0(k,r) = (E_n(k - A(r)) + \Phi(r))P_I(k)$$

and, using the φ corresponding to (16), we obtain that the Berry connection coefficient $\mathcal{A}_1(k) = -\mathrm{i}/(2\pi)\,\langle \varphi_n(k), \partial_{k_1}\varphi_n(k)\rangle$ is a periodic function of k_2 and independent of k_1. Hence, introducing the kinetic momentum $\tilde{k} := k - A(r)$ and, recalling that $A(r) = A_1(r)\gamma_1^*$, we have $\mathscr{A}_1(\tilde{k}) = \mathscr{A}_1(k)$. Using this and specializing to the case $\Gamma = \mathbb{Z}^2$ for the moment, one finds for the subprincipal symbol of

$$\mathfrak{h} = u \sharp \pi \sharp H \sharp \pi \sharp u^* = P_I \sharp u \sharp H \sharp u^* \sharp P_I,$$

by the same reasoning as in the proof of [Teufel 2003, Corollary 5.12], the expression

$$\begin{aligned}\mathfrak{h}_1(k,r) = \Big(-\mathscr{A}_1(\tilde{k})(\partial_2 E_n(\tilde{k})B(r) - \partial_{r_1} E_n(\tilde{k})) + (\mathscr{A}_2(k) - \mathscr{A}_2(\tilde{k}))(\partial_2\Phi(r)\\ - \partial_1 E_n(\tilde{k})B(r)) + B(r)\,\mathrm{Re}\big(\mathrm{i}\big\langle\partial_1\varphi_n(\tilde{k}), (H_{\mathrm{per}} - E_n)(\tilde{k})\partial_2\varphi_n(\tilde{k})\big\rangle_{\mathscr{H}_{\mathrm{f}}}\big)\Big)P_I(k)\\ - \tfrac{1}{2}\mathrm{i}\nabla_r(E_n(\tilde{k}) + \Phi(r))M(k),\end{aligned}$$

where $\tilde{k} := k - A(r)$ and $B = \operatorname{curl} A = \partial_2 A_1$. Using $P_I(k)\nabla P_I(k)P_I(k) = 0$, the last term in $\mathfrak{h}_1$ cancels exactly $h_{1,\mathrm{c}}$ in h_1 and we find

$$\begin{aligned}h_1^{\mathrm{eff}}(k,r) &= \langle\varphi_n(k), h_1(k,r)\varphi_n(k)\rangle\\ &= -\mathscr{A}_1(\tilde{k})(\partial_2 E_n(\tilde{k})B(r) - \partial_{r_1}E_n(\tilde{k})) + (\mathscr{A}_2(k) - \mathscr{A}_2(\tilde{k}))(\partial_2\Phi(r) - \partial_1 E_n(\tilde{k})B(r)) + B(r)\mathscr{M}(\tilde{k}),\end{aligned}$$

with

$$\mathscr{M}(\tilde{k}) := \mathrm{Re}\big(\mathrm{i}\langle\partial_1\varphi_n(\tilde{k}), (H_{\mathrm{per}} - E_n)(\tilde{k})\partial_2\varphi_n(\tilde{k})\rangle_{\mathscr{H}_{\mathrm{f}}}\big)$$

the Rammal–Wilkinson term. To get a nicer expression we compute the symbol with respect to the θ-quantization. According to Proposition 6.14 we have to add

$$\begin{aligned}-\bigg(\mathscr{A}_1(k)\partial_{r_1}h_0^{\mathrm{eff}}(k,r) + \bigg(\mathscr{A}_2(k) - \frac{\theta k_1}{2\pi}\bigg)\partial_{r_2}h_0^{\mathrm{eff}}(k,r)\bigg)\\ = -\mathscr{A}_1(k)(\partial_{r_1}E_n(\tilde{k}) + \partial_1\Phi(r)) - \bigg(\mathscr{A}_2(k) - \frac{\theta k_1}{2\pi}\bigg)(\partial_2\Phi(r) - \partial_1 E_n(\tilde{k})B(r)).\end{aligned}$$

In summary we have

$$h_1^{\mathrm{eff},\theta}(k,r) = -\mathscr{A}_1(\tilde{k})(\partial_1\Phi(r) + \partial_2 E_n(\tilde{k})B(r)) - \bigg(\mathscr{A}_2(\tilde{k}) - \frac{\theta k_1}{2\pi}\bigg)(\partial_2\Phi(r) - \partial_1 E_n(\tilde{k})B(r)) + B(r)\mathscr{M}(\tilde{k}),$$

where we note that the combination $\mathscr{A}_2(\tilde{k}) - \theta k_1/(2\pi)$ is a Γ^*-periodic function.

So, in summary, we obtain the following corollary:

Corollary 5.2. *Let Assumptions 1 and 2 hold with $A^{(1)} = 0$ and let $E(k) \equiv E_n(k)$ be an isolated nondegenerate Bloch band. Then there is a Γ^*-periodic symbol $h^{\mathrm{eff},\theta} \in S^1(\varepsilon, \mathscr{L}(\mathbb{C}))$ such that, for the effective Hamiltonian $H_n^{\mathrm{eff}} := H_{I=\{n\}}^{\mathrm{eff}}$ from Theorem 5.1, it holds that*

$$\|H_n^{\mathrm{eff}} - \mathrm{Op}^\theta(h^{\mathrm{eff},\theta})\|_{\mathscr{L}(\mathscr{H}_\alpha)} = \mathcal{O}(\varepsilon^\infty). \tag{25}$$

The asymptotic expansion of the symbol $h^{\mathrm{eff},\theta}$ can be computed, in principle, to any order in ε. Its principal symbol is given by

$$h_0(k,r) = E(\tilde{k}) + \Phi(r),$$

and its subprincipal symbol by

$$h_1(k,r) = \mathcal{A}(k,r)\cdot(B(r)\nabla E(\tilde{k})^{\perp} - \nabla\Phi(r)) + B(r)\mathcal{M}(\tilde{k}),$$

where $\tilde{k} := k - A(r)$, $\nabla E(\tilde{k})^{\perp} = (-\partial_2 E(\tilde{k}), \partial_1 E(\tilde{k}))$ *and*

$$\mathcal{M}(k) = -\operatorname{Im}\big(\langle\partial_1\varphi(k), (H_{\mathrm{per}} - E)(k)\partial_2\varphi(k)\rangle_{\mathcal{H}_{\mathrm{f}}}\big).$$

The Berry connection coefficient $\mathcal{A}$ *is given by*

$$\mathcal{A}(k,r) = \mathcal{A}_1(\tilde{k})\gamma_1 + \Big(\mathcal{A}_2(\tilde{k}) - \frac{\theta}{2\pi}\langle k,\gamma_1\rangle\Big)\gamma_2,$$

where the components $\mathcal{A}_j$ *are computed from the function* φ *constructed in Proposition 4.2 as*

$$\mathcal{A}_j(k) = -\frac{\mathrm{i}}{2\pi}\langle\varphi(k), \partial_{\kappa_j}\varphi(k)\rangle := -\frac{\mathrm{i}}{2\pi}\langle\varphi(k), \gamma_j^*\cdot\nabla\varphi(k)\rangle.$$

The two terms in the subprincipal symbol have the following physical meaning: Since $\nabla E_n(k)$ is the velocity of a particle with quasimomentum k in the n-th band, the term in brackets is the Lorentz force on the particle. Since the θ-quantization takes into account the integrated curvature of the Berry connection of $2\pi\theta$ per lattice cell of Γ^*, the curvature form of the effective Berry connection coefficient $\mathcal{A}$ integrates to zero. The second term in h_1 is a correction to the energy, known as the Rammal–Wilkinson term. For the case $\theta = 0$ we recover the first-order correction to Peierls substitution established in [Panati et al. 2003a].

6. Weyl quantization on the Bloch bundle

In this section we construct quantization schemes that map suitable symbols to pseudodifferential operators that act on sections of possibly nontrivial bundles. Our construction is related to and motivated by similar constructions in the literature [Pflaum 1998a; 1998b; Safarov 1997; Sharafutdinov 2004; 2005; Hansen 2011]. As opposed to the case of functions on $\mathbb{R}^n$, the relation between a pseudodifferential operator acting on sections of a vector bundle and its symbol becomes more subtle. If one defines a corresponding pseudodifferential calculus in local coordinates, as is done in [Hörmander 1985], for example, one can associate a symbol to an operator which is unique only up to an error of order ε. To define a full symbol, one has to take into account the geometry of the vector bundle. This means that instead of local coordinates, one must use a connection on the vector bundle and a connection on the base space. This idea goes back to Widom [1978; 1980], who was the first to develop a complete isomorphism between such pseudodifferential operators and their symbols. However, while he showed how to recover the full symbol from a pseudodifferential operator and proved that this map is bijective, he did not provide an explicit integral formula for the quantization map. His work was developed further by Pflaum [1998b] and Safarov [1997]. Pflaum [1998b] constructs a quantization map which maps symbols that are sections of endomorphism bundles to operators between the sections of the corresponding bundles. In his quantization formulas he uses a cutoff function so that he can use the exponential map corresponding to a given connection on the manifold that may not be defined globally. A geometric symbol calculus for pseudodifferential operators between sections of vector bundles can also be found in [Sharafutdinov 2004; 2005], where the author moreover introduces the notion of a geometric symbol in comparison to a coordinatewise symbol. A semiclassical variant of this calculus can be found in [Hansen 2011]. When we compute the symbol f such that $\mathrm{Op}^\tau(\mathfrak{f}) = \mathrm{Op}^{\mathrm{B}}(f) + \mathbb{O}(\varepsilon^\infty)$, one could say, using the language of [Sharafutdinov 2004; 2005], that f is the geometric symbol with respect to the Berry connection of the operator $\mathrm{Op}^\tau(\mathfrak{f})$.

While Safarov [1997] and Pflaum [1998a] provide formulas for the Weyl quantization, this is done only for pseudodifferential operators on manifolds and not for operators between sections of vector bundles. Moreover, Safarov and Pflaum consider only Hörmander symbol classes [1985]. In the following we define semiclassical Weyl calculi for more general symbol classes and include the case of bundles with an infinite-dimensional Hilbert space as the typical fiber. In addition we prove a Calderón–Vaillancourt-type theorem establishing L^2-boundedness and provide explicit formulas relating the different symbols of an operator corresponding to different quantization maps. However, our constructions are specific to bundles over the torus. Requiring periodicity conditions for symbols and functions allows us to project the calculus from the cover $\mathbb{R}^2$ to the quotient $\mathbb{R}^2/\mathbb{Z}^2$, an approach already used in [Gérard and Nier 1998; Panati et al. 2003a; Teufel 2003]. A similar approach was also applied in [Asch et al. 1994], where the authors consider the Bochner Laplacian acting on sections of a line bundle with connection over the torus. In our calculus, the Bochner Laplacian $-\Delta_k$ corresponding to a connection is obtained by quantization of the symbol $f(k,r) = r^2$ for $\varepsilon = 1$ using the same connection.

The Berry quantization. The basic idea of the "Berry quantization" is to map multiplication by r to the covariant derivative $\mathrm{i}\varepsilon\nabla_k^{\mathrm{B}}$. In contrast to the τ-quantization, where r is mapped to $\mathrm{i}\varepsilon\nabla_k$, this has two advantages. Since $\mathrm{i}\varepsilon\nabla_k^{\mathrm{B}}$ is a connection on the Bloch bundle, it leaves invariant its space of sections. As a consequence, $f(k, \mathrm{i}\varepsilon\nabla_k^{\mathrm{B}})$ commutes with P_I if and only if $f(k,r)$ commutes with $P_I(k)$ for all $(k,r) \in M^* \times \mathbb{R}^2$. Moreover, the connection ∇_k^{B} restricted to sections of the Bloch bundle is unitarily equivalent to the connection ∇_k^α on the bundle Ξ_α via the unitary map U_α.

As in [Panati et al. 2003a; Teufel 2003], a symbol $f_\varepsilon \in S^w(\varepsilon, \mathcal{L}(\mathcal{H}_{\mathrm{f}}))$ is called τ-equivariant (more precisely, (τ_1, τ_2)-equivariant) if

$$f_\varepsilon(q-\gamma, p) = \tau_2(\gamma) f_\varepsilon(q,p) \tau_1(\gamma)^{-1} \quad \text{for all } \gamma \in \Gamma.$$

The spaces of τ-equivariant symbols are denoted by $S^w_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_{\mathrm{f}}))$.

Using the parallel transport $t^{\mathrm{B}}(x,y)$ with respect to the Berry connection introduced in Lemma 4.1, we define the Berry quantization $\mathrm{Op}^{\mathrm{B}}_\chi(f) \in \mathcal{L}(\mathcal{H}_\tau)$ for τ-equivariant symbols $f \in S^1_\tau(\mathcal{L}(\mathcal{H}_{\mathrm{f}}))$ as

$$(\mathrm{Op}^{\mathrm{B}}_\chi(f)\psi)(k) = \frac{1}{(2\pi\varepsilon)^2} \int_{\mathbb{R}^2} \biggl(\int_{\mathbb{R}^2} \mathrm{e}^{\mathrm{i}(k-y)r/\varepsilon} \chi(k-y) t^{\mathrm{B}}\bigl(k, \tfrac{1}{2}(k+y)\bigr) f\bigl(\tfrac{1}{2}(k+y), r\bigr) t^{\mathrm{B}}\bigl(\tfrac{1}{2}(k+y), y\bigr) \psi(y)\,\mathrm{d}y \biggr) \mathrm{d}r. \quad (26)$$

Here, in contrast to the usual Weyl quantization rule, we take into account that ψ is a section of a vector bundle with connection ∇^{B} and that the symbol $f(\,\cdot\,, r)$ is really a section of its endomorphism bundle. So, for $f\bigl(\frac{1}{2}(k+y), r\bigr)$ to act on $\psi(y)$ we first need to map $\psi(y)$ into the correct fiber of the bundle, which is done by the parallel transport $t^{\mathrm{B}}\big(\frac{1}{2}(k+y), y\big)$. However, since the derivatives of $t^{\mathrm{B}}(x, y)$ are not uniformly bounded, we introduce a cutoff function χ in the definition. The choice of this cutoff function has only an effect of order $\mathbb{O}(\varepsilon^\infty)$ on the operator, but it simplifies the following analysis considerably.

Definition 6.1. A function $\chi \in C^\infty(\mathbb{R}^2)$ is called a smooth cutoff function if supp χ is compact, $\chi \equiv 1$ in a neighborhood of 0, and $0 \le \chi \le 1$.

Since we need $\mathrm{Op}^{\mathrm{B}}_\chi(f)$ only for $f \in S^1_\tau(\mathcal{L}(\mathcal{H}_{\mathrm{f}}))$ as an operator on $\mathcal{H}_\tau$, we do not follow the usual routine and show that it is well defined on distributions for general symbol classes. We also do not develop a full Moyal calculus for products of such pseudodifferential operators, although this could be done easily with the tools we provide.

For all steps the following simple lemma will be crucial. It states that the cutoff function in the definition of $\mathrm{Op}^{\mathrm{B}}_\chi(f)$ ensures that all derivatives of the parallel transport in the integral remain bounded uniformly.

Lemma 6.2. *There are constants c_α such that*

$$\|\partial_x^\alpha t^{\mathrm{B}}(x, y)\| \le c_\alpha \quad \textit{for all } x, y \in \mathbb{R}^2 \textit{ with } |x-y| < 1.$$

Proof. This follows from the smoothness of t^{B} and its τ-equivariance (13). ☐

Before we prove $\mathcal{H}_\tau$-boundedness we first show that $\mathrm{Op}^{\mathrm{B}}_\chi(f)$ is well defined on smooth functions.

Proposition 6.3. *Let $f \in S^1_\tau(\mathcal{L}(\mathcal{H}_{\mathrm{f}}))$ and $\psi \in C^\infty(\mathbb{R}^2, \mathcal{H}_{\mathrm{f}}) \cap \mathcal{H}_\tau$. Then $\mathrm{Op}^{\mathrm{B}}_\chi(f)\psi \in C^\infty(\mathbb{R}^2, \mathcal{H}_{\mathrm{f}}) \cap \mathcal{H}_\tau$.*

Proof. First note that, because of the cutoff function, the y-integral in (26) extends only over a bounded region. Thus one can use

$$\mathrm{e}^{-\mathrm{i}y\cdot r/\varepsilon} = \left(\frac{1-\varepsilon^2\Delta_y}{1+r^2}\right)^N \mathrm{e}^{-\mathrm{i}y\cdot r/\varepsilon}$$

and integration by parts in order to show r-integrability of the inner integral. Therefore $(\mathrm{Op}^{\mathrm{B}}_\chi(f)\psi)(k)$ is well defined and its smoothness follows immediately, since, by dominated convergence, we can differentiate under the integral and still get enough decay in r by the above trick. The τ-equivariance of $(\mathrm{Op}^{\mathrm{B}}_\chi(f)\psi)(k)$ can be checked directly using the τ-equivariance of ψ, t^{B} and f. ☐

Proposition 6.4. *Let $f \in S^1_\tau(\mathcal{L}(\mathcal{H}_{\mathrm{f}}))$. Then $\mathrm{Op}^{\mathrm{B}}_\chi(f) \in \mathcal{L}(\mathcal{H}_\tau)$ with*

$$\|\mathrm{Op}^{\mathrm{B}}_\chi(f)\|_{\mathcal{L}(\mathcal{H}_\tau)} \le c_\chi \|f\|_{\infty,(4,1)},$$

where the constant c_χ depends only on χ and

$$\|f\|_{\infty,(4,1)} := \sum_{|\beta|\le 4, |\beta'|\le 1} \sup_{k\in M^*, r\in\mathbb{R}^2} \|\partial_k^\beta \partial_r^{\beta'} f(k, r)\|_\infty.$$

Proof. Let $\tilde\chi : \mathbb{R}^2 \to [0, 1]$ be a cutoff function such that supp$\tilde\chi \subset \{|r| < 1\}$ and $\sum_{j\in\mathbb{Z}^2} \tilde\chi_j(r) \equiv 1$, where $\tilde\chi_j(r) := \tilde\chi(r-j)$, and let $f_j := \tilde\chi_j f$. If we can show that $\mathrm{Op}^{\mathrm{B}}_\chi(f_j) \in \mathcal{L}(\mathcal{H}_\tau)$ and

$$\sup_{j\in\mathbb{Z}^2} \sum_{i\in\mathbb{Z}^2} \|\mathrm{Op}^{\mathrm{B}}_\chi(f_j)^* \mathrm{Op}^{\mathrm{B}}_\chi(f_i)\|^{1/2}_{\mathcal{L}(\mathcal{H}_\tau)} \le M \quad \text{and} \quad \sup_{j\in\mathbb{Z}^2} \sum_{i\in\mathbb{Z}^2} \|\mathrm{Op}^{\mathrm{B}}_\chi(f_j)\, \mathrm{Op}^{\mathrm{B}}_\chi(f_i)^*\|^{1/2}_{\mathcal{L}(\mathcal{H}_\tau)} \le M, \tag{27}$$

then, according to the Cotlar–Stein lemma — see [Dimassi and Sjöstrand 1999, Lemma 7.10] — it follows that $\sum_{j\in\mathbb{Z}^2}\mathrm{Op}^{\mathrm{B}}_\chi(f_j)$ converges strongly to a bounded operator $F\in\mathcal{L}(\mathcal{H}_\tau)$ with $\|F\|_{\mathcal{L}(\mathcal{H}_\tau)}\le M$. However, the following lemma shows that $F=\mathrm{Op}^{\mathrm{B}}_\chi(f)$:

Lemma 6.5. *If $\psi\in C^\infty(\mathbb{R}^2, C^\infty(\mathbb{R}^2,\mathcal{H}_{\mathrm{f}})\cap\mathcal{H}_\tau$ then there is a constant C such that, for all $f\in S^1_\tau(\mathcal{L}(\mathcal{H}_{\mathrm{f}}))$ with* supp $f\subset\mathbb{R}^2\times\{|r|>R\}$,

$$\|\mathrm{Op}^{\mathrm{B}}_\chi(f)\psi(k)\|_{\mathcal{H}_{\mathrm{f}}}\le\frac{C}{R^2}\|f\|_{\infty,(4,0)}.$$

Proof. Proceed as in the proof of Proposition 6.3, using

$$\mathrm{e}^{-\mathrm{i}y\cdot r/\varepsilon}=\frac{\varepsilon^4}{r^4}\Delta_y^2\mathrm{e}^{-\mathrm{i}y\cdot r/\varepsilon}$$

instead. □

Hence, on the dense set $\psi\in C^\infty(\mathbb{R}^2,\mathcal{H}_{\mathrm{f}})\cap\mathcal{H}_\tau$ the sequence $\sum_j\mathrm{Op}^{\mathrm{B}}_\chi(f_j)\psi$ converges uniformly and thus also in the norm of $\mathcal{H}_\tau$ to $\mathrm{Op}^{\mathrm{B}}_\chi(f)\psi$.

So we are left to show (27), which follows immediately once we can show

$$\|\mathrm{Op}^{\mathrm{B}}_\chi(f_j)^*\,\mathrm{Op}^{\mathrm{B}}_\chi(f_i)\|_{\mathcal{L}(\mathcal{H}_\tau)}\le C(|i-j|+1)^{-4}\|f_i\|_{\infty,(4,1)}\|f_j\|_{\infty,(4,1)} \tag{28}$$

and the analogous second bound for all $i,j\in\mathbb{Z}^2$. Let $\phi,\psi\in\mathcal{H}_\tau$; then

$$\begin{aligned}&\langle\phi,\mathrm{Op}^{\mathrm{B}}_\chi(f_j)^*\,\mathrm{Op}^{\mathrm{B}}_\chi(f_i)\psi\rangle_{\mathcal{H}_\tau}\\&=\frac{1}{(2\pi\varepsilon)^4}\int_{M^*}\mathrm{d}q\int_{\mathbb{R}^8}\mathrm{d}y\,\mathrm{d}k\,\mathrm{d}r\,\mathrm{d}r'\,\mathrm{e}^{\mathrm{i}k(r-r')/\varepsilon}\mathrm{e}^{\mathrm{i}(qr'-yr)/\varepsilon}\chi(q-k)\chi(k-y)\phi^*(q)t^{\mathrm{B}}\big(k,\tfrac12(q+k)\big)\\&\qquad\times f_j^*\big(\tfrac12(q+k),r'\big)t^{\mathrm{B}}\big(\tfrac12(q+k),k\big)t^{\mathrm{B}}\big(k,\tfrac12(k+y)\big)f_i\big(\tfrac12(k+y),r\big)t^{\mathrm{B}}\big(\tfrac12(k+y),y\big)\psi(y).\end{aligned}$$

Because of the cutoff functions, the domains of integration for k and y are also restricted to compact convex sets $M^*\subset M_k\subset M_y$, respectively.

For $|i-j|>2$, f_i and f_j have disjoint r-support and

$$\mathrm{e}^{\mathrm{i}k\cdot(r-r')/\varepsilon}=\left(\frac{-\varepsilon^2\Delta_k}{|r-r'|^2}\right)^2\mathrm{e}^{\mathrm{i}k\cdot(r-r')/\varepsilon}\quad\text{for } r-r'\neq0.$$

Now we insert this into the above integral, integrate by parts, take the norm into the integral and obtain, for $|i-j|>2$,

$$\begin{aligned}&|\langle\phi,\mathrm{Op}^{\mathrm{B}}_\chi(f_j)^*\,\mathrm{Op}^{\mathrm{B}}_\chi(f_i)\psi\rangle|\\&\le\frac{\varepsilon^4}{(2\pi\varepsilon)^4}\int_{M^*}\mathrm{d}q\int_{M_k}\mathrm{d}k\int_{M_y}\mathrm{d}y\int_{\mathbb{R}^4}\mathrm{d}r\,\mathrm{d}r'\,\frac{1}{|r-r'|^4}\sum_{\beta_1,\dots,\beta_8}|\partial_k^{\beta_1}\chi(q-k)||\partial_k^{\beta_2}\chi(k-y)|\\&\quad\times\|\phi^*(q)\|\,\big\|\partial_k^{\beta_3}t^{\mathrm{B}}\big(k,\tfrac12(q+k)\big)\big\|\,\big\|\partial_k^{\beta_4}f_j^*\big(\tfrac12(q+k),r'\big)\big\|\,\big\|\partial_k^{\beta_5}t^{\mathrm{B}}\big(\tfrac12(q+k),k\big)\big\|\,\big\|\partial_k^{\beta_6}t^{\mathrm{B}}\big(k,\tfrac12(k+y)\big)\big\|\\&\qquad\times\big\|\partial_k^{\beta_7}f_i\big(\tfrac12(k+y),r\big)\big\|\,\big\|\partial_k^{\beta_8}t^{\mathrm{B}}\big(\tfrac12(k+y),y\big)\big\|\,\|\psi(y)\|\end{aligned}$$

$$\leq c\|f_j\|_{\infty,4}\|f_i\|_{\infty,4}\sum_{\beta_1,\beta_2}\int_{M^*}\mathrm{d}q\int_{M_k}\mathrm{d}k\int_{M_y}\mathrm{d}y\int_{\operatorname{supp}\tilde{\chi}_i}\mathrm{d}r\int_{\operatorname{supp}\tilde{\chi}_j}\mathrm{d}r'$$
$$\times\frac{\|\phi(q)\|\|\psi(y)\|}{|r-r'|^4}|\partial_k^{\beta_1}\chi(q-k)||\partial_k^{\beta_2}\chi(k-y)|.$$

Here the sum $\sum_{\beta_1,\dots,\beta_8}$ runs over a finite number of multi-indices and we used Lemma 6.2. Moreover, we have that, because of the τ-equivariance,

$$\|f_j\|_{\infty,4}:=\sum_{|\beta|\leq 4}\sup_{\substack{k\in M_y\\ r\in\mathbb{R}^2}}\|\partial_k^\beta f_j(k,r)\|=\sum_{|\beta|\leq 4}\sup_{\substack{k\in M^*\\ r\in\mathbb{R}^2}}\|\partial_k^\beta f(k,r)\|.$$

For the remaining integral we get

$$\int_{M^*}\mathrm{d}q\int_{M_k}\mathrm{d}k\int_{M_y}\mathrm{d}y\int_{\operatorname{supp}\tilde{\chi}_i}\mathrm{d}r\int_{\operatorname{supp}\tilde{\chi}_j}\mathrm{d}r'\,\frac{\|\phi(q)\|\|\psi(y)\|}{|r-r'|^4}|\partial_k^{\beta_1}\chi(q-k)||\partial_k^{\beta_2}\chi(k-y)|$$
$$\leq\frac{c_2}{(|i-j|-2)^4}\int_{M_k}\mathrm{d}k\,(\|\phi_{M^*}\|*\partial_k^{\beta_1}\chi)(k)(\|\psi_{M_y}\|*\partial_k^{\beta_2}\chi)(k)$$
$$\leq\frac{c_2}{(|i-j|-2)^4}\|\phi_{M^*}\|_2\|\psi_{M_y}\|_2\|\partial_k^{\beta_1}\chi\|_1\|\partial_k^{\beta_2}\chi\|_1$$
$$\leq\frac{c_3}{(|i-j|-2)^4}\|\phi\|_{\mathcal{H}_\tau}\|\psi\|_{\mathcal{H}_\tau},$$

where we used the Cauchy–Schwarz and Young inequalities in the next-to-last step. Here $\phi_{M^*}(q):=\phi(q)\mathbf{1}_{M^*}(q)$ and $\psi_{M_y}(q):=\psi(q)\mathbf{1}_{M_y}(q)$.

In order to obtain a bound uniform in ε on $\|\mathrm{Op}^{\mathrm{B}}_\chi(f_j)^*\,\mathrm{Op}^{\mathrm{B}}_\chi(f_i)\|_{\mathcal{H}_\tau}$ for all i and j directly, observe that one can get the factor $\varepsilon^4/(|r-r'|^2|k-y||q-k|)$ from appropriate integrations by parts also in r and r', using

$$\mathrm{e}^{\mathrm{i}(k-y)\cdot r/\varepsilon}=\frac{-\mathrm{i}\varepsilon(k-y)\cdot\nabla_r}{|k-y|^2}\mathrm{e}^{\mathrm{i}(k-y)\cdot r/\varepsilon}.$$

The remaining expression can be bounded as before, noting that $1/|r-r'|^2$ is integrable on $\mathbb{R}^4$ and that $\partial_k^\beta\chi(k)/|k|$ is integrable on $\mathbb{R}^2$. In summary, we can conclude (28), which finishes the proof. □

Next we check that the choice of the cutoff function only has an effect of order $\mathcal{O}(\varepsilon^\infty)$.

Proposition 6.6. *Let $f\in S^1_\tau(\mathcal{L}(\mathcal{H}_\mathrm{f}))$ and let χ_1 and χ_2 be two cutoff functions. Then*

$$\|\mathrm{Op}^{\mathrm{B}}_{\chi_1}(f)-\mathrm{Op}^{\mathrm{B}}_{\chi_2}(f)\|=\mathcal{O}(\varepsilon^\infty).$$

Proof. Let $\overline{\chi}:=\chi_1-\chi_2$; then $0<c\leq|k|\leq C<\infty$ for all $k\in\operatorname{supp}\chi$. We control the norm of $\mathrm{Op}^{\mathrm{B}}_{\overline{\chi}}(f)=\mathrm{Op}^{\mathrm{B}}_{\chi_1}(f)-\mathrm{Op}^{\mathrm{B}}_{\chi_2}(f)$ as in the previous proof. So we have to estimate the integrals

$$\langle\phi,\mathrm{Op}^{\mathrm{B}}_{\overline{\chi}}(f_j)^*\,\mathrm{Op}^{\mathrm{B}}_{\overline{\chi}}(f_i)\psi\rangle_{\mathcal{H}_\tau}$$
$$=\frac{1}{(2\pi\varepsilon)^4}\int_{M^*}\mathrm{d}q\int_{\mathbb{R}^8}\mathrm{d}y\,\mathrm{d}k\,\mathrm{d}r\,\mathrm{d}r'\,\mathrm{e}^{\mathrm{i}(k-y)\cdot r/\varepsilon}\mathrm{e}^{\mathrm{i}(q-k)\cdot r'/\varepsilon}\overline{\chi}(q-k)\overline{\chi}(k-y)\phi^*(q)t^{\mathrm{B}}\big(k,\tfrac{1}{2}(q+k)\big)$$
$$\times f_j^*\big(\tfrac{1}{2}(q+k),r'\big)t^{\mathrm{B}}\big(\tfrac{1}{2}(q+k),k\big)t^{\mathrm{B}}\big(k,\tfrac{1}{2}(k+y)\big)f_i\big(\tfrac{1}{2}(k+y),r\big)t^{\mathrm{B}}\big(\tfrac{1}{2}(k+y),y\big)\psi(y).$$

Using

$$\mathrm{e}^{\mathrm{i}(k-y)\cdot r/\varepsilon} = \left(\frac{-\varepsilon^2\Delta_r}{|k-y|^2}\right)^N \mathrm{e}^{\mathrm{i}(k-y)\cdot r/\varepsilon} \quad \text{for } k-y \neq 0,$$

we can get any power of ε^2 by integration by parts and estimating the remaining expression as in the previous proof. □

In the following we drop the subscript χ in $\mathrm{Op}^{\mathrm{B}}_\chi(f)$ in the notation whenever the statement is not affected by a change of order ε^∞. Also note that $\mathrm{Op}^\tau(f) - \mathrm{Op}^\tau_\chi(f) = \mathcal{O}(\varepsilon^\infty)$ for any cutoff function χ.

Next we relate the τ- and the Berry quantization by using a Taylor expansion of the parallel transport.

Lemma 6.7. *For $\delta \in \mathbb{R}^2$ with $|\delta| < \delta_0$ small enough, the parallel transport from z to $z+\delta$ has a uniformly and absolutely convergent expansion*

$$t^{\mathrm{B}}(z+\delta, z) = \sum_{n=0}^\infty t_n^{i_1,\dots,i_n}(z)\delta_{i_1}\cdots\delta_{i_n} := \sum_{n=0}^\infty \sum_{(i_1,\dots,i_n)\in\{1,2\}^n} t_n^{i_1,\dots,i_n}(z)\delta_{i_1}\cdots\delta_{i_n},$$

where the coefficients $t_n^{i_1,\dots,i_n} : \mathbb{R}^2 \to \mathcal{L}(\mathcal{H}_\mathrm{f})$ are real-analytic and τ-equivariant. The first terms are, explicitly,

$$t_0 = \mathbf{1}_{\mathcal{H}_\mathrm{f}} \quad \textit{and} \quad t_1(z) = M(z) := [\nabla P_I(z), P_I(z)].$$

Proof. Note that $t^{\mathrm{B}}(z+\delta, z) = t(1)$, where $t(s)$ is the solution of

$$\frac{\mathrm{d}}{\mathrm{d}s}t(s) = [\delta\cdot\nabla P_I(z+s\delta), P_I(z+s\delta)]t(s) =: \delta\cdot M(z+s\delta)t(s) \quad \text{with} \quad t(0) = \mathbf{1}.$$

Since $\delta\cdot M : \mathbb{R}^2 \to \mathcal{L}(\mathcal{H}_\mathrm{f})$ is smooth and uniformly bounded, the solution of this linear ODE is given by the uniformly convergent Dyson series

$$\begin{aligned} &t^{\mathrm{B}}(z+\delta, z) - \mathbf{1} \\ &\quad= \sum_{n=1}^\infty \int_0^1 \int_0^{t_1} \cdots \int_0^{t_{n-1}} \delta\cdot M(z+t_1\delta)\cdots\delta\cdot M(z+t_n\delta)\,\mathrm{d}t_n\cdots\mathrm{d}t_1 \\ &\quad= \sum_{n=1}^\infty \int_0^1 \int_0^{t_1} \cdots \int_0^{t_{n-1}} \sum_{m_1=0}^\infty \cdots \sum_{m_n=0}^\infty \frac{t_1^{m_1}(\delta\cdot\nabla)^{m_1}\delta\cdot M(z)}{m_1!}\cdots\frac{t_n^{m_n}(\delta\cdot\nabla)^{m_n}\delta\cdot M(z)}{m_n!}\,\mathrm{d}t_n\cdots\mathrm{d}t_1, \end{aligned}$$

where in the second equality we inserted the uniformly convergent power series for the real-analytic function $\delta\cdot M$,

$$\delta\cdot M(z+t\delta) = \sum_{m=0}^\infty \frac{t^m(\delta\cdot\nabla)^m\delta\cdot M(z)}{m!}. \qquad \square$$

Theorem 6.8. *Let $f \in S^1_\tau(\mathcal{L}(\mathcal{H}_\mathrm{f}))$ and define, for $n \in \mathbb{N}_0$,*

$$\mathfrak{f}_n(k,r) := \sum_{\substack{a,b\in\mathbb{N}_0\\ a+b=n}} \frac{(-1)^a}{(2\mathrm{i})^n} t_a^{i_1,\dots,i_a}(k)(\partial_{r_{i_1}}\cdots\partial_{r_{i_a}}\partial_{r_{j_1}}\cdots\partial_{r_{j_b}} f)(k,r)(t_b^{j_1,\dots,j_b}(k))^*.$$

Then $\mathfrak{f}_n \in S^1_\tau(\mathcal{L}(\mathcal{H}_\mathrm{f}))$ *and*

$$\Big\| \sum_{n=0}^{N} \varepsilon^n \operatorname{Op}^\tau(\mathfrak{f}_n) - \operatorname{Op}^\mathrm{B}(f) \Big\|_{\mathcal{L}(\mathcal{H}_\tau)} = \mathcal{O}(\varepsilon^{N+1}). \tag{29}$$

The first terms are, explicitly, $\mathfrak{f}_0(k, r) = f(k, r)$ *and*

$$\mathfrak{f}_1(k, r) = \tfrac{1}{2}\mathrm{i}(\nabla_r f(k, r) \cdot M(k) + M(k) \cdot \nabla_r f(k, r)),$$

where $M(k) = [\nabla P_I(k), P_I(k)]$. *Moreover, if* f *has compact* r*-support, then*

$$\lim_{N\to\infty} \sum_{n=0}^{N} \varepsilon^n \operatorname{Op}^\tau_\chi(\mathfrak{f}_n) = \operatorname{Op}^\mathrm{B}_\chi(f)$$

strongly in $\mathcal{H}_\tau$.

Proof. The idea is to insert the Taylor expansion of t^B from Lemma 6.7 into the integral in the definition (26). To this end first note that, with $\delta := \frac{1}{2}(k - y)$, we have that

$$t^\mathrm{B}\big(k, \tfrac{1}{2}(k + y)\big) = t^\mathrm{B}\big(\tfrac{1}{2}(k + y) + \delta, \tfrac{1}{2}(k + y)\big) \quad \text{and} \quad t^\mathrm{B}\big(\tfrac{1}{2}(k + y), y\big) = t^\mathrm{B}\big(\tfrac{1}{2}(k + y) - \delta, \tfrac{1}{2}(k + y)\big)^*.$$

Assume that f has compact r-support for the moment. Then for $\psi \in \mathcal{H}_\tau$ we get

$$\begin{aligned}
(\operatorname{Op}^\mathrm{B}_\chi(f)\psi)(k) &= \frac{1}{(2\pi\varepsilon)^2} \int_{\mathbb{R}^4} \mathrm{d}y\, \mathrm{d}r\, \mathrm{e}^{\mathrm{i}2\delta\cdot r/\varepsilon} \chi(k - y) \sum_{a=0}^{\infty} t_a^{i_1,\dots,i_a}\big(\tfrac{1}{2}(k + y)\big)\delta_{i_1} \cdots \delta_{i_a} f\big(\tfrac{1}{2}(k + y), r\big) \\
&\qquad \times \sum_{b=0}^{\infty} (-1)^b t_b^{j_1,\dots,j_b}\big(\tfrac{1}{2}(k + y)\big)^* \delta_{j_1} \cdots \delta_{j_b} \psi(y) \\
&= \frac{1}{(2\pi\varepsilon)^2} \sum_{a,b=0}^{\infty} (-1)^b \int_{\mathbb{R}^4} \mathrm{d}y\, \mathrm{d}r \left(\frac{\varepsilon}{2\mathrm{i}}\right)^{a+b} (\partial_{r_{i_1}} \cdots \partial_{r_{i_a}} \partial_{r_{j_1}} \cdots \partial_{r_{j_b}} \mathrm{e}^{\mathrm{i}2\delta\cdot r/\varepsilon}) \\
&\qquad \times \chi(k - y) t_a^{i_1,\dots,i_a}\big(\tfrac{1}{2}(k + y)\big) f\big(\tfrac{1}{2}(k + y), r\big) t_b^{j_1,\dots,j_b}\big(\tfrac{1}{2}(k + y)\big)^* \psi(y) \\
&= \frac{1}{(2\pi\varepsilon)^2} \sum_{a,b=0}^{\infty} (-1)^a \left(\frac{\varepsilon}{2\mathrm{i}}\right)^{a+b} \int_{\mathbb{R}^4} \mathrm{d}y\, \mathrm{d}r\, \mathrm{e}^{\mathrm{i}(k-y)\cdot r/\varepsilon} \chi(k - y) t_a^{i_1,\dots,i_a}\big(\tfrac{1}{2}(k + y)\big) \\
&\qquad \times (\partial_{r_{i_1}} \cdots \partial_{r_{i_a}} \partial_{r_{j_1}} \cdots \partial_{r_{j_b}} f)\big(\tfrac{1}{2}(k + y), r\big) t_b^{j_1,\dots,j_b}\big(\tfrac{1}{2}(k + y)\big)^* \psi(y) \\
&= \sum_{n=0}^{\infty} \varepsilon^n (\operatorname{Op}^\tau_\chi(\mathfrak{f}_n)\psi)(k).
\end{aligned}$$

Here we used that all sums and integrals converge absolutely and uniformly, so interchanging sums and integrals is no problem. Moreover, by the fact that $\operatorname{Op}^\mathrm{B}_\chi(f)\psi$ is a uniformly bounded and τ-equivariant function, the pointwise convergence implies also the strong convergence in $\mathcal{H}_\tau$.

In order to estimate $\Delta_N\psi := \big(\sum_{n=0}^{N-1}\varepsilon^n \operatorname{Op}^\tau_\chi(\mathfrak{f}_n) - \operatorname{Op}^{\mathrm{B}}_\chi(f)\big)\psi$ in $\mathcal{H}_\tau$, we estimate, as in the previous proofs, $|\langle\phi, \Delta_N\psi\rangle|$. Write, for the remainder in the Taylor expansion,

$$\begin{aligned} t^{\mathrm{B}}(z+\delta, z) &= \sum_{a=0}^{N-1} t_a^{i_1,\dots,i_a}(z)\delta_{i_1}\cdots\delta_{i_a} + \frac{(\partial_{i_1}\cdots\partial_{i_N} t^{\mathrm{B}})(z+\xi(\delta)\delta, z)}{N!}\delta_{i_1}\cdots\delta_{i_N} \\ &=: \sum_{a=0}^{N-1} t_a^{i_1,\dots,i_a}(z)\delta_{i_1}\cdots\delta_{i_a} + R_N^{i_1,\dots,i_N}(z,\delta)\delta_{i_1}\cdots\delta_{i_N}; \end{aligned}$$

then one term appearing in the estimate of $|\langle\phi, \Delta_N\psi\rangle|$ is

$$\begin{aligned} &\frac{1}{(2\pi\varepsilon)^2}\int_{M^*}\mathrm{d}k\int_{\mathbb{R}^4}\mathrm{d}y\,\mathrm{d}r\,\mathrm{e}^{\mathrm{i}2\delta\cdot r/\varepsilon}\chi(k-y)\phi^*(k)R_N^{i_1,\dots,i_N}\big(\tfrac12(k+y),\delta\big)\delta_{i_1}\cdots\delta_{i_N} f\big(\tfrac12(k+y),r\big)\psi(y) \\ &\quad= \frac{1}{(2\pi\varepsilon)^2}\left(\frac{-\varepsilon}{2\mathrm{i}}\right)^N\int_{M^*}\mathrm{d}k\int_{\mathbb{R}^4}\mathrm{d}y\,\mathrm{d}r\,\mathrm{e}^{\mathrm{i}(k-y)\cdot r/\varepsilon}\chi(k-y)\phi^*(k)R_N^{i_1,\dots,i_N}\big(\tfrac12(k+y),\delta\big) \\ &\qquad\qquad\times(\partial_{r_{i_1}}\cdots\partial_{r_{i_N}} f)\big(\tfrac12(k+y),r\big)\psi(y). \end{aligned}$$

Such an expression can be bounded by a constant times $\varepsilon^N\|\phi\|\|\psi\|$ by obtaining an integrable factor $\varepsilon^2/(|r||k-y|)$ through additional integration by parts, as in the proof of Proposition 6.4. All other terms can be treated similarly, so we have shown (29) for f with compact r-support.

For the general statement we use again the Cotlar–Stein lemma on the family of almost orthogonal operators $\Delta_{N,i} := \sum_{n=0}^{N-1}\varepsilon^n \operatorname{Op}^\tau_\chi(\mathfrak{f}_{n,i}) - \operatorname{Op}^{\mathrm{B}}_\chi(f_i)$. While this is very lengthy to write down, the estimates are completely analogous to those of Proposition 6.4, using integration by parts as before. □

Of course, we can reverse the roles of the two quantizations and obtain the reverse statement.

Corollary 6.9. *Let* $\mathfrak{f} \in S^1_\tau(\mathcal{L}(\mathcal{H}_\mathrm{f}))$ *and define*

$$f_n(k,r) := \sum_{a+b=n}\frac{(-1)^a}{(2\mathrm{i})^n}(t_a^{i_1,\dots,i_a}(k))^*(\partial_{r_{i_1}}\cdots\partial_{r_{i_a}}\partial_{r_{j_1}}\cdots\partial_{r_{j_b}}\mathfrak{f})(k,r)t_b^{j_1,\dots,j_b}(k) \quad \textit{for } n\in\mathbb{N}_0.$$

Then $f_n \in S^1_\tau(\mathbb{R}^4, \mathcal{L}(\mathcal{H}_\mathrm{f}))$ *and*

$$\Big\|\sum_{n=0}^{N}\varepsilon^n \operatorname{Op}^{\mathrm{B}}(f_n) - \operatorname{Op}^\tau(\mathfrak{f})\Big\|_{\mathcal{L}(\mathcal{H}_\tau)} = \mathcal{O}(\varepsilon^{N+1}).$$

The first terms are, explicitly, $f_0(k,r) = \mathfrak{f}(k,r)$ *and*

$$f_1(k,r) = -\tfrac12(\mathrm{i})(\nabla_r\mathfrak{f}(k,r)\cdot M(k) + M(k)\cdot\nabla_r\mathfrak{f}(k,r)).$$

While we do not use the following proposition explicitly, it sheds some light on the geometric significance of the Berry quantization. It states that $\operatorname{Op}^{\mathrm{B}}(f)$ commutes with the projection P_I if and only if the symbol $f(k,r)$ commutes pointwise with $P_I(k)$.

Proposition 6.10. *Let* $f \in S^1_\tau(\mathcal{L}(\mathcal{H}_\mathrm{f}))$. *Then*

$$[f(k,r), P_I(k)] = 0 \quad \textit{for all } (k,r)\in\mathbb{R}^4 \qquad \Longleftrightarrow \qquad [\operatorname{Op}^{\mathrm{B}}(f), P_I] = 0.$$

Proof. It suffices to consider the commutator on the dense set $C^\infty(\mathbb{R}^2, \mathcal{H}_\mathrm{f}) \cap \mathcal{H}_\tau$, so we can work with the integral definition (26) of $\mathrm{Op}^\mathrm{B}(f)$. For $\psi \in C^\infty(\mathbb{R}^2, \mathcal{H}_\mathrm{f}) \cap \mathcal{H}_\tau$ it follows from (12) that

$$
\begin{aligned}
&([\mathrm{Op}^\mathrm{B}_\chi(f), P_I]\psi)(k) \\
&= \frac{1}{(2\pi)^2} \\
&\quad \times \int_{\mathbb{R}^2} \biggl(\int_{\mathbb{R}^2} \mathrm{e}^{\mathrm{i}(k-y)r} \chi(k-y) t^\mathrm{B}\bigl(k, \tfrac{1}{2}(k+y)\bigr) \bigl[f\bigl(\tfrac{1}{2}(k+y), \varepsilon r\bigr), P_I\bigl(\tfrac{1}{2}(k+y)\bigr)\bigr] t^\mathrm{B}\bigl(\tfrac{1}{2}(k+y), y\bigr) \psi(y)\, \mathrm{d}y \biggr) \mathrm{d}r
\end{aligned}
$$

so the implication from left to right is obvious. To prove the reverse implication in detail is somewhat tedious. Since we don't use it, we only sketch the argument. Assume that $[f(k,r), P_I(k)] = O(k,r) \neq 0$. Then $O \in S^1_\tau(\mathbb{R}^4, \mathcal{L}(\mathcal{H}_\mathrm{f}))$ and one can show that $\|\mathrm{Op}^\mathrm{B}_\chi(O)\| \geq C > 0$ for some C independent of ε by looking at the action of $\mathrm{Op}^\mathrm{B}_\chi(O)$ on suitable coherent states. This even implies the stronger statement

$$[\mathrm{Op}^\mathrm{B}(f), P_I] = o(\varepsilon) \quad \Longrightarrow \quad [f(k,r), P_I(k)] = 0 \quad \text{for all } (k,r) \in \mathbb{R}^4. \qquad \square$$

The α-quantization and the θ-quantization. The other two quantizations we use are the α-quantization and the effective quantization. The α-quantization with respect to the connection $\nabla^\alpha = U_\alpha \nabla^\mathrm{B} U^*_\alpha$ is used to map α-equivariant symbols in $C^\infty(\mathbb{R}^4, \mathcal{L}(\mathbb{C}^m))$ to operators in $\mathcal{L}(\mathcal{H}_\alpha)$; see Definition 4.4. For $m = 1$ it can be replaced by the effective quantization with respect to the explicit connection $\nabla^\theta_k := \nabla_k + \mathrm{i}\theta/(2\pi)\, \langle k, \gamma_1\rangle \gamma_2$.

In both cases the construction is exactly the same as the one for the Berry quantization, which is to use the parallel transport of the desired connection in the definition of the quantization. Let

$$t^\alpha(x,y) : \mathbb{C}^m \to \mathbb{C}^m, \quad \lambda \mapsto t^\alpha(x,y)\lambda := U_\alpha(x) t^\mathrm{B}(x,y) U^*_\alpha(y)\lambda,$$

be the parallel transport along the straight line from y to x with respect to the connection $\nabla^\alpha = U_\alpha \nabla^\mathrm{B} U^*_\alpha$. Then τ-equivariance of t^B implies α-equivariance of t^α, i.e.,

$$t^\alpha(x-\gamma^*, y-\gamma^*) = \alpha\biggl(\frac{\langle x, \gamma_2\rangle}{2\pi}\biggr)^{-n_1} t^\alpha(x,y) \alpha\biggl(\frac{\langle y, \gamma_2\rangle}{2\pi}\biggr)^{n_1}.$$

For $m = 1$ we introduce the effective connection $\nabla^\theta_k = \nabla_k + \mathrm{i}\theta/(2\pi)\, \langle k, \gamma_1\rangle \gamma_2$ and the corresponding α-equivariant parallel transport

$$t^\theta(x,y) : \mathbb{C} \to \mathbb{C}, \quad \lambda \mapsto t^\theta(x,y)\lambda := \mathrm{e}^{(\mathrm{i}\theta/(4\pi))\langle x+y, \gamma_1\rangle \langle y-x, \gamma_2\rangle}\lambda.$$

We say that a symbol $f \in C^\infty(\mathbb{R}^4, \mathcal{L}(\mathbb{C}^m))$ is α-equivariant if

$$f(k-\gamma^*, r) = \alpha(\kappa_2)^{-n_1} f(k,r) \alpha(\kappa_2)^{n_1} \quad \text{for all } \gamma^* \in \Gamma^*,\ k, r \in \mathbb{R}^2,$$

where we again use the notation $\kappa_j = \langle k, \gamma_j\rangle/(2\pi)$. Note that for $m = 1$ the α-equivariant symbols are just the periodic symbols. However, for $m > 1$ the κ_2-derivatives of an α-equivariant symbol are in general unbounded as functions of κ_1. Thus we define the space of "bounded" symbols $S_\alpha(\mathcal{L}(\mathbb{C}^m))$ as follows:

Definition 6.11. Let $S_\alpha(\mathscr{L}(\mathbb{C}^m))$ be the space of α-equivariant functions $f \in C^\infty(\mathbb{R}^4, \mathscr{L}(\mathbb{C}^m))$ that satisfy

$$\sup_{k\in M^*, r\in\mathbb{R}^2} \|(\partial_k^\alpha \partial_r^\beta f)(k,r)\|_{\mathscr{L}(\mathbb{C}^m)} < \infty \quad \text{for all } \alpha, \beta \in \mathbb{N}_0^2.$$

As always, $S_\alpha(\mathscr{L}(\mathbb{C}^m))$ is equipped with the corresponding Fréchet metric and $S_\alpha(\varepsilon, \mathscr{L}(\mathbb{C}^m))$ denotes the space of uniformly bounded functions $f : [0, \varepsilon_0) \to S_\alpha(\mathscr{L}(\mathbb{C}^m))$.

In complete analogy to the Berry quantization, we define for α-equivariant symbols $f \in S_\alpha(\mathscr{L}(\mathbb{C}^m))$ and $\psi \in \mathscr{H}_\alpha$ the α-quantization by

$$(\mathrm{Op}_\chi^\alpha(f)\psi)(k) := \frac{1}{(2\pi\varepsilon)^2}\int_{\mathbb{R}^2}\left(\int_{\mathbb{R}^2} \mathrm{e}^{\mathrm{i}(k-y)r/\varepsilon}\chi(k-y)t^\alpha\big(k, \tfrac12(k+y)\big) f\big(\tfrac12(k+y), r\big) t^\alpha\big(\tfrac12(k+y), y\big)\psi(y)\,\mathrm{d}y\right)\mathrm{d}r,$$

and, for $m = 1$, the θ-quantization by

$$\begin{aligned}(\mathrm{Op}_\chi^\theta(f)\psi)(k) &:= \frac{1}{(2\pi\varepsilon)^2}\int_{\mathbb{R}^2}\left(\int_{\mathbb{R}^2} \mathrm{e}^{\mathrm{i}(k-y)r/\varepsilon}\chi(k-y)t^\theta\big(k, \tfrac12(k+y)\big) f\big(\tfrac12(k+y), r\big) t^\theta\big(\tfrac12(k+y), y\big)\psi(y)\,\mathrm{d}y\right)\mathrm{d}r \\ &= \frac{1}{(2\pi\varepsilon)^2}\int_{\mathbb{R}^2}\left(\int_{\mathbb{R}^2} \mathrm{e}^{\mathrm{i}(k-y)r/\varepsilon}\chi(k-y)\mathrm{e}^{\mathrm{i}\theta/(4\pi)\langle x+y,\gamma_1\rangle\langle y-x,\gamma_2\rangle} f\big(\tfrac12(k+y), r\big)\psi(y)\,\mathrm{d}y\right)\mathrm{d}r.\end{aligned}$$

Now we can show all results of the previous section in a completely analogous way also for the α- and the θ-quantizations.

Proposition 6.12. *Let $f \in S_\alpha(\mathbb{R}^4, \mathscr{L}(\mathbb{C}^m))$. Then $\mathrm{Op}_\chi^\alpha(f) \in \mathscr{L}(\mathscr{H}_\alpha)$, with*

$$\|\mathrm{Op}_\chi^\alpha(f)\|_{\mathscr{L}(\mathscr{H}_\alpha)} \le c_\chi \|f\|_{\infty,(4,1)} := c_\chi \sum_{\substack{|\beta|\le 4\\ |\beta'|\le 1}} \sup_{\substack{k\in M^*\\ r\in\mathbb{R}^2}} \|\partial_k^\beta \partial_r^{\beta'} f(k,r)\|,$$

where the constant c_χ depends only on χ. For $m = 1$ the same bound holds for $\mathrm{Op}_\chi^\theta(f)$.

Proposition 6.13. *Let $f \in S_\tau^1(\mathscr{L}(\mathscr{H}_\mathrm{f}))$ and*

$$f_I(k,r)_{ij} := \langle \varphi_i(k), f(k,r)\varphi_j(k)\rangle.$$

Then $f_I \in S_\alpha(\mathbb{C}^m)$ and

$$\mathrm{Op}_\chi^\alpha(f_I) = U_\alpha \,\mathrm{Op}_\chi^\mathrm{B}(f) U_\alpha^*.$$

Proof. It follows directly from the definitions that $f_I \in S_\alpha(\mathbb{C}^m)$. The equality of the operators can be checked on the dense set $C^\infty(\mathbb{R}^2) \cap \mathscr{H}_\alpha$ using their integral definitions and the fact that, again by definition, $U_\alpha^*(x)t^\alpha(x,y) = t^\mathrm{B}(x,y)U_\alpha^*(y)$. □

For the case $m = 1$ we can finally replace the α- by the θ-quantization if we suitably modify the symbol. To this end we introduce the Taylor series of the difference of the parallel transports as

$$t^{\theta *}(k, k+\delta)t^\alpha(k, k+\delta) =: \sum_{n=0}^\infty t_n^{i_1,\dots,i_n}(k)\delta_{i_1}\cdots\delta_{i_n},$$

where

$$t_0(k) \equiv 1 \quad \text{and} \quad t_1(k) = \mathrm{i}\Big(\mathscr{A}_1(k)\gamma_1 + \Big(\mathscr{A}_2(k) - \frac{\theta}{2\pi}\langle k, \gamma_1\rangle\Big)\gamma_2\Big) =: \mathrm{i}\mathscr{A}(k).$$

The proof of the following proposition is analogous to the proof of Theorem 6.8. The expressions simplify a bit because for $m = 1$ the symbol and the parallel transport commute.

Proposition 6.14. *Let $f \in S^1(\mathbb{R}^4, \mathbb{C})$ be a periodic symbol and define, for $n \in \mathbb{N}_0$,*

$$f_n^\theta(k, r) := \mathrm{i}^n t_n^{i_1,\dots,i_n}(k)(\partial_{r_{i_1}} \cdots \partial_{r_{i_n}} f)(k, r).$$

Then $f_n^\theta \in S^1(\mathbb{R}^4, \mathbb{C})$ is periodic and

$$\Big\| \sum_{n=0}^{N} \varepsilon^n \operatorname{Op}^\theta(f_n^\theta) - \operatorname{Op}^\alpha(f) \Big\|_{\mathscr{L}(\mathscr{H}_\alpha)} = \mathcal{O}(\varepsilon^{N+1}). \tag{30}$$

The first terms are, explicitly, $f_0^\theta(k, r) = f(k, r)$ and

$$f_1^\theta(k, r) = -\mathscr{A}(k) \cdot \nabla_r f(k, r).$$

7. Application to the Hofstadter model

In this section we apply the general theory developed in the previous sections to perturbations of magnetic subbands of the Hofstadter Hamiltonian [1976]. The motivation for doing this is twofold. First it shows, in the simplest possible example, how magnetic Peierls substitution Hamiltonians can be explicitly computed and analyzed. Second, we will find strong support for the conjecture that Theorem 5.1 is actually still valid for perturbations by small constant fields B. Note that the Hofstadter Hamiltonian and related tight-binding models served not only as model Hamiltonians for the illustration of general results on perturbed periodic Schrödinger operators but also gave rise to considerable mathematical work dedicated specifically to them, e.g., [Helffer and Sjöstrand 1989; 1990a; Helffer et al. 1990; Bellissard et al. 1991; Avila and Jitomirskaya 2009]. For a recent overview of the mathematics and the physics literature on the Hofstadter Hamiltonian we refer to [De Nittis 2010].

The Hofstadter model is the canonical model for a single nonmagnetic Bloch band perturbed by a constant magnetic field B_0. It can be seen to arise from the tight-binding formalism in physics or, alternatively, from Peierls substitution for a nonmagnetic Bloch band. The Hofstadter Hamiltonian is the discrete magnetic Laplacian on the lattice $\widetilde{\Gamma} = \mathbb{Z}^2$,

$$H_{\mathrm{Hof}}^{B_0} = D_1 + D_1^* + D_2 + D_2^* \quad \text{acting on } \ell^2(\mathbb{Z}^2).$$

Here D_1 and D_2 are the (dual) magnetic translations

$$(D_1\psi)(x) := \psi(x - e_1) \quad \text{and} \quad (D_2\psi)(x) := \mathrm{e}^{\mathrm{i}B_0\langle x, e_1\rangle}\psi(x - e_2).$$

For $B_0 = 2\pi p/q$ we define the corresponding magnetic Bloch–Floquet transformation on the lattice $\Gamma = q\mathbb{Z} \times \mathbb{Z}$ as

$$\mathcal{U}_{\mathrm{BF}} : \ell^2(\Gamma; \mathbb{C}^q) \to L^2(\mathbb{T}^*_q; \mathbb{C}^q), \quad (\mathcal{U}_{\mathrm{BF}}\psi)(k)_j := \sum_{\gamma\in\Gamma} \mathrm{e}^{\mathrm{i}\gamma\cdot k}(T_\gamma\psi)((j,0)) \quad \text{for } j = 0, \dots, q-1,$$

where we recall that the magnetic translations T_γ were defined in (5). Note that the fiber space $\mathcal{H}_{\mathrm{f}} = \mathbb{C}^q$ is now finite-dimensional and thus we can drop the additional phase $\mathrm{e}^{-\mathrm{i}k\cdot y}$ in the definition of $\mathcal{U}_{\mathrm{BF}}$, which appeared in (7) to make the domain of $H_{\mathrm{per}}(k)$ independent of k. As a consequence, the range of $\mathcal{U}_{\mathrm{BF}}$ now contains periodic functions on $\mathbb{T}^*_q = [0, 2\pi/q) \times [0, 2\pi)$ and τ-equivariance becomes periodicity. A straightforward computation shows that the shift operators D_j become matrix-multiplication operators $\widehat{D}_j := \mathcal{U}_{\mathrm{BF}} D_j \mathcal{U}^*_{\mathrm{BF}}$,

$$\widehat{D}_1(k) = \begin{pmatrix} 0 & 0 & 0 & \cdots & \mathrm{e}^{\mathrm{i}qk_1} \\ 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{pmatrix} \quad \text{and} \quad \widehat{D}_2(k) = \mathrm{e}^{\mathrm{i}k_2} \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & \mathrm{e}^{\mathrm{i}B_0} & 0 & \cdots & 0 \\ 0 & 0 & \mathrm{e}^{\mathrm{i}2B_0} & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & 0 \\ 0 & 0 & \cdots & 0 & \mathrm{e}^{\mathrm{i}(q-1)B_0} \end{pmatrix}.$$

For the Hamiltonian one thus finds

$$\widehat{H}^{B_0}_{\mathrm{Hof}}(k) = \begin{pmatrix} 2\cos(k_2) & 1 & 0 & \dots & \mathrm{e}^{\mathrm{i}qk_1} \\ 1 & 2\cos(k_2 - B_0) & 1 & \dots & 0 \\ 0 & 1 & 2\cos(k_2 - 2B_0) & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & & & & 1 \\ \mathrm{e}^{-\mathrm{i}qk_1} & 0 & \dots & 1 & 2\cos(k_2 - (q-1)B_0) \end{pmatrix},$$

which is indeed $2\pi/q$-periodic in k_1 and 2π-periodic in k_2. The spectrum of $\widehat{H}^{B_0}_{\mathrm{Hof}}(k)$ consists of q distinct eigenvalue bands $E_n(k)$, $n = 1, \dots, q$, with periodic spectral projections $P_n(k)$, defining the magnetic Bloch bands and Bloch bundles of the Hofstadter model. The spectrum of $H^{B_0}_{\mathrm{Hof}}$ is the union of the ranges of the functions $E_n(k)$ and thus consists of q intervals. As a function of B_0, the spectrum is depicted in the famous Hofstadter butterfly (Figure 2). Note that for $B_0 \notin 2\pi\mathbb{Q}$ the spectrum of $H^{B_0}_{\mathrm{Hof}}$ is a Cantor-type set, that is, a nowhere dense, closed set of Lebesgue measure zero; see [Avila and Jitomirskaya 2009].

Osadchy and Avron [2001] produced a colored version of the butterfly by coloring the gaps in the spectrum according to the sum of the Chern numbers of the overlying bands; see Figure 3. For example, for $B_0 = 2\pi\frac{1}{3}$, the top and the bottom bands have Chern number 1 each and the middle band has Chern number -2. Thus the gaps are labeled from top to bottom by 0 (white), 1 (red), -1 (blue), and again 0 (white).

Now we apply the machinery developed in the previous sections to determine Peierls substitution Hamiltonians for magnetic subbands of $H^{B_0}_{\mathrm{Hof}}$. Let $B_0 = 2\pi p/q$; then $\widehat{H}^{B_0}_{\mathrm{Hof}}(k)$ is a matrix-valued function on the torus $\mathbb{T}^*_q = [0, 2\pi/q) \times [0, 2\pi)$, but its eigenvalue bands have period $2\pi/q$ in both directions.

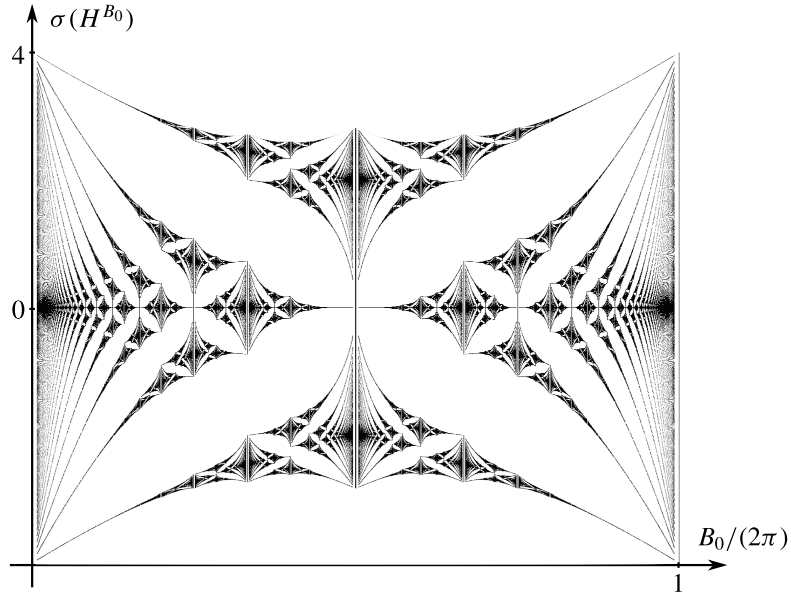

Figure 2. The black and white butterfly [Hofstadter 1976] showing the spectrum of $H^{B_0}_{\mathrm{Hof}}$ as a function of B_0. For rational values $B_0 = 2\pi p/q$ the spectrum of $H^{B_0}_{\mathrm{Hof}}$ consists of q disjoint intervals if q is odd and of $q-1$ disjoint intervals if q is even.

Hence we can take as a model dispersion relation

$$E_q(k) := 2(\cos(qk_1) + \cos(qk_2)) = \mathrm{e}^{\mathrm{i}qk_1} + \mathrm{e}^{-\mathrm{i}qk_1} + \mathrm{e}^{\mathrm{i}qk_2} + \mathrm{e}^{-\mathrm{i}qk_2}.$$

This is, up to a constant factor, the leading-order part in the Fourier expansion of any Bloch band $E_n(k)$ on $\mathbb{T}^*_q$. So we pick an isolated simple subband of $\widehat{H}^{B_0}_{\mathrm{Hof}}(k)$ with Chern number $\theta \in \mathbb{Z}$ and approximate its dispersion by $E_q(k)$. If we now perturb B_0 by an additional "small" constant magnetic field $B = \operatorname{curl} A(x)$ with $A(x) = (0, Bx_1)$, the Peierls substitution Hamiltonian for this subband is given as the θ-quantization of $E_q(k - A(r))$,

$$H^B_{\theta,q} := \mathrm{Op}^\theta(E_q(k - A(r))) = \mathrm{e}^{\mathrm{i}q\mathcal{K}_1} + \mathrm{e}^{-\mathrm{i}q\mathcal{K}_1} + \mathrm{e}^{\mathrm{i}q\mathcal{K}_2} + \mathrm{e}^{-\mathrm{i}q\mathcal{K}_2},$$

with

$$\mathcal{K}_1 = k_1 \quad \text{and} \quad \mathcal{K}_2 = k_2 - \mathrm{i}B\nabla^\theta_1 = k_2 - \mathrm{i}B\partial_{k_1}$$

acting on

$$\mathcal{H}_\theta = \{f \in L^2_{\mathrm{loc}}(\mathbb{R}^2) \mid f(k_1 - 2\pi/q, k_2) = \mathrm{e}^{\mathrm{i}\theta k_2} f(k_1, k_2) \text{ and } f(k_1, k_2 - 2\pi) = f(k_1, k_2)\}.$$

Here $\nabla^\theta_k = (\partial_{k_1}, \partial_{k_2} + \mathrm{i}q\theta k_1/(2\pi))$ and, due to our choice of gauge for the perturbing magnetic field, the operator $H^B_{\theta,q}$ depends on θ only through its domain. Note that this gauge is different from the one used in Theorem 5.1 and we use it to simplify the analysis of the resulting operator $H^B_{\theta,q}$. However, since Theorem 5.1 does not cover the case of a perturbation by a constant magnetic field anyway, our derivation of $H^B_{\theta,q}$ is merely heuristic for any choice of gauge.

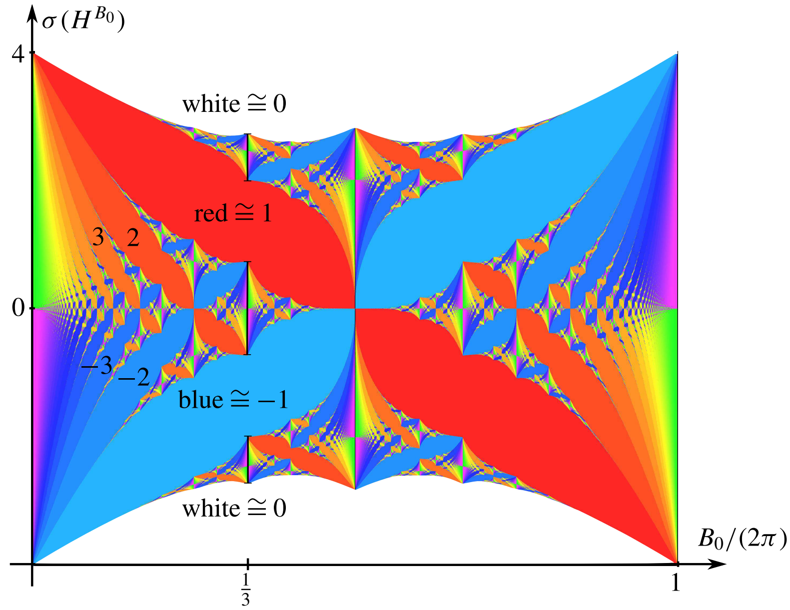

Figure 3. The colored butterfly for the Hofstadter Hamiltonian $H_{\text{Hof}}^{B_0}$, as first plotted in [Osadchy and Avron 2001]. The colored regions are open components of the resolvent set and the colors encode Chern numbers of overlying Bloch bundles. Physically, the Chern numbers represent the Hall conductivity of a corresponding noninteracting Fermi gas. For fixed B_0, i.e., in each vertical line, the Chern numbers of the single bands sum up to the total Chern number $\theta = 0$, as represented by the white region on bottom of the butterfly.

To determine the spectrum of $H_{\theta,q}^{B}$, it is sufficient to notice that it has the structure

$$U_1 + U_1^* + U_2 + U_2^*$$

with unitary operators U_1 and U_2 that satisfy

$$U_1 U_2 = \mathrm{e}^{\mathrm{i}q^2 B} U_2 U_1 =: \mathrm{e}^{\mathrm{i}\alpha} U_2 U_1. \tag{31}$$

The C^*-algebra $\mathcal{N}_\alpha$ generated by two abstract elements $\mathfrak{U}_1$ and $\mathfrak{U}_2$ satisfying (31) is called the noncommutative torus. The mappings

$$\pi_{\theta,q}^{B} : \mathcal{N}_{q^2 B} \to \mathcal{L}(\mathcal{H}_\theta), \quad \mathfrak{U}_j \mapsto \mathrm{e}^{\mathrm{i}q\mathcal{X}_j},$$

thus define a $*$-representation of $\mathcal{N}_{q^2 B}$ into the bounded operators on $\mathcal{H}_\theta$. Accordingly, each operator $H_{\theta,q}^{B}$ is a representation of the abstract element $\mathfrak{H}^\alpha = \mathfrak{U}_1 + \mathfrak{U}_1^* + \mathfrak{U}_2 + \mathfrak{U}_2^*$ of $\mathcal{N}_\alpha$ for $\alpha = q^2 B$. Since one can show that the representations $\pi_{\theta,q}^{B}$ are $*$-isomorphisms onto their ranges (see [De Nittis 2010; Freund 2013; Amr et al. 2015]), this implies that the spectrum of $H_{\theta,q}^{B}$ agrees with the spectrum of $\mathfrak{H}^{q^2 B}$. However, the latter is just the spectrum of $H_{\text{Hof}}^{q^2 B}$, i.e., it is again given by the black and white Hofstadter butterfly.

In order to associate Chern numbers with the spectral subbands of $H^B_{\theta,q}$, we now turn it by a suitable unitary transformation into matrix-multiplication form. Since $H^B_{\theta,q}$ contains within $\mathrm{e}^{\mathrm{i}q\mathcal{K}_2}$ a shift by qB in the k_1-direction, this is possible if we assume this shift to be a rational fraction of the width $2\pi/q$ of the Brillouin zone, that is, $qB = (2\pi/q)\tilde{p}/\tilde{q}$ or $B = (2\pi/q^2)\tilde{p}/\tilde{q}$ with $\tilde{p}$ and $\tilde{q}$ coprime. To this end we pass from $\mathcal{H}_\theta$, i.e., from complex-valued functions on the Brillouin zone $M^*_q = [0, 2\pi/q) \times [0, 2\pi)$, to $\mathbb{C}^{\tilde{q}}$-valued functions on the further reduced Brillouin zone $M^*_{q,\tilde{q}} = [0, 2\pi/(q\tilde{q})) \times [0, 2\pi)$. To define the corresponding unitary map $U^B : \mathcal{H}_\theta \to L^2(M^*_{q,\tilde{q}}, \mathbb{C}^{\tilde{q}})$, we let

$$M_j := \{(k_1, k_2) \in M^*_q \mid k_1 \in [(j-1)qB, (j-1)qB + 2\pi/(q\tilde{q}))\} \quad \text{for } j = 1, \dots, \tilde{q}$$

and define

$$(U^B\psi)_j(k) := \mathrm{e}^{\mathrm{i}\theta k_2 (j-1)\tilde{p}/\tilde{q}} \psi(k_1 + (j-1)qB, k_2) \quad \text{for } k \in M^*_{q,\tilde{q}}.$$

Thus $(U^B\psi)_j$ is obtained by restricting $\psi \in \mathcal{H}_\theta$ to the region M_j, translating it to $M^*_{q,\tilde{q}} = M_1$ and finally multiplying it by $\mathrm{e}^{\mathrm{i}\theta k_2 (j-1)\tilde{p}/\tilde{q}}$. The last phase turns the translation by qB in the k_1-direction on $\mathcal{H}_\theta$ into the cyclic permutation of components in $L^2(M^*_{q,\tilde{q}}, \mathbb{C}^{\tilde{q}})$ multiplied by a phase. More precisely, we have

$$\mathrm{e}^{\mathrm{i}q\mathcal{K}_1}\psi(k) = \mathrm{e}^{\mathrm{i}qk_1}\psi(k_1, k_2) \quad \text{and thus} \quad (U^B \mathrm{e}^{\mathrm{i}q\mathcal{K}_1}\psi)_j(k) = \mathrm{e}^{\mathrm{i}q(k_1 + (j-1)qB)}\psi_j(k),$$

and

$$\mathrm{e}^{\mathrm{i}q\mathcal{K}_2}\psi(k) = \mathrm{e}^{\mathrm{i}qk_2}\psi(k_1 + qB, k_2) \quad \text{and thus} \quad (U^B \mathrm{e}^{\mathrm{i}q\mathcal{K}_2}\psi)_j(k) = \mathrm{e}^{\mathrm{i}qk_2}\mathrm{e}^{-\mathrm{i}\theta k_2 \tilde{p}/\tilde{q}}\psi_{j+1}(k).$$

Hence $U^B H^B_{\theta,q} U^{B*}$ acts as the matrix-valued multiplication operator

$$H^B_{\theta,q}(k) = \begin{pmatrix} 2\cos(qk_1) & \mathrm{e}^{\mathrm{i}k_2(q-\theta\tilde{p}/\tilde{q})} & 0 & \dots & \mathrm{e}^{-\mathrm{i}k_2(q-\theta\tilde{p}/\tilde{q})} \\ \mathrm{e}^{-\mathrm{i}k_2(q-\theta\tilde{p}/\tilde{q})} & 2\cos(q(k_1+qB)) & \mathrm{e}^{\mathrm{i}k_2(q-\theta\tilde{p}/\tilde{q})} & \dots & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}k_2(q-\theta\tilde{p}/\tilde{q})} & 2\cos(q(k_1+2qB)) & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & & & & \mathrm{e}^{\mathrm{i}k_2(q-\theta\tilde{p}/\tilde{q})} \\ \mathrm{e}^{\mathrm{i}k_2(q-\theta\tilde{p}/\tilde{q})} & 0 & \dots & \mathrm{e}^{-\mathrm{i}k_2(q-\theta\tilde{p}/\tilde{q})} & 2\cos(q(k_1+(\tilde{q}-1)qB)) \end{pmatrix}. \tag{32}$$

Like the Hofstadter matrix $\widehat{H}^{B_0}_{\mathrm{Hof}}(k)$, also $H^B_{\theta,q}(k)$ has $\tilde{q}$ distinct eigenvalue bands $E^B_{\theta,q,n}(k)$, $n = 1, \dots, \tilde{q}$. By the isospectrality of $H^B_{\theta,q}$ and $H^{q^2B}_{\mathrm{Hof}}$, the ranges of these band functions all agree. However, as functions they are, in general, distinct. The corresponding eigenprojections $P^B_{\theta,q,n}(k)$ define line bundles over the torus $M^*_{q,\tilde{q}}$ and one can compute their Chern numbers by integrating the curvature of the corresponding Berry connection $P^B_{\theta,q,n} U^B \nabla^\theta_k U^{B*}$ over the reduced Brillouin zone $M^*_{q,\tilde{q}}$. Using a program from [Amr 2015], we did this numerically for a large number of values for θ, q and B and found that the Chern numbers of the subbands of $H^B_{\theta,q}(k)$ always match the Chern numbers of the corresponding sub-subbands of the Hofstadter Hamiltonian. To make this more precise, recall that $H^B_{\theta,q}(k)$ was derived as the Peierls substitution Hamiltonian for a magnetic subband of $H^{B_0}_{\mathrm{Hof}}$ for $B_0 = 2\pi p/q$ with Chern number θ perturbed by a small additional magnetic field B. The Chern numbers of the subbands of $H^B_{\theta,q}(k)$ for

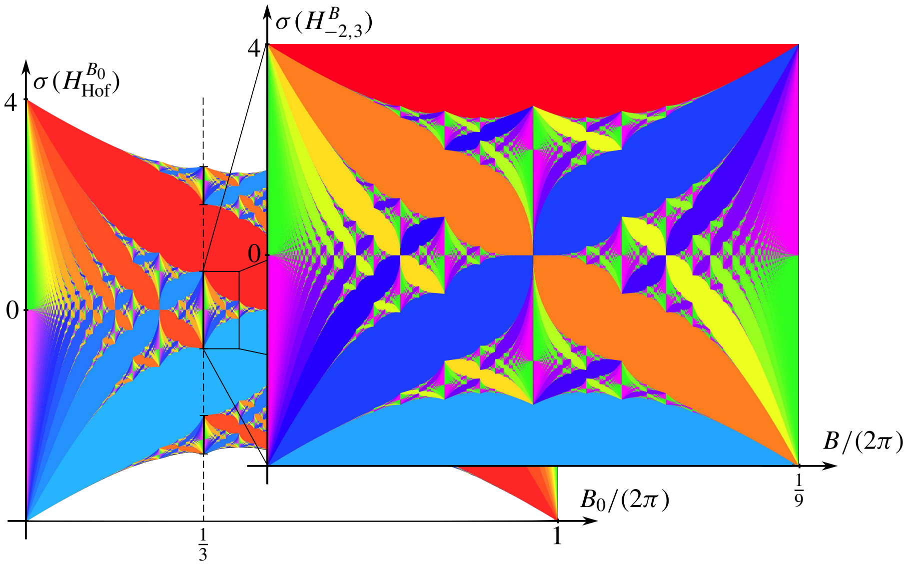

Figure 4. The operator $H^{B}_{-2,3}$ is up to a constant factor and higher-order terms in the Fourier expansion of $E_2(k)$ the leading order part of the Peierls substitution Hamiltonian for the middle band of $H^{B_0}_{\mathrm{Hof}}$ for $B_0 = 2\pi\frac{1}{3}$. This band has Chern number -2. As can be seen from the coloring, the Chern numbers of the subbands of $H^{B}_{-2,3}$ for $B/(2\pi) \in \left[0, \frac{1}{9}\right]$ exactly match the Chern numbers of the corresponding subbands of $H^{B_0+\widetilde{B}}_{\mathrm{Hof}}$, where $\widetilde{B} = B\bigl(1 - 1/(1+\pi/(3B))\bigr) = B(1+\mathbb{O}(B))$.

$B = (2\pi/q^2)\tilde{p}/\tilde{q}$ agree with the Chern numbers of the subbands of $H^{B_0+\widetilde{B}}_{\mathrm{Hof}}$ into which the unperturbed subband of $H^{B_0}_{\mathrm{Hof}}$ splits. Here

$$\widetilde{B} = B\left(1 - \frac{1}{1 - 2\pi/(q\theta B)}\right) = B\left(1 - \frac{1}{1 - q\tilde{q}/(\theta\tilde{p})}\right) = B + \mathbb{O}(B^2).$$

The situation is depicted in Figure 4. Note, however, that for drawing the colored butterfly of $H^{B}_{\theta,q}$ it is not feasible to compute all Chern numbers numerically by integrating the curvature of the Berry connection. This is because, for large denominators $\tilde{q}$, the matrix $H^{B}_{\theta,q}(k)$ and the number of its subbands becomes large. Instead, in [Amr 2015] an algorithm was found that allows to compute the Chern numbers of $H^{B}_{\theta,q}$ in a purely algebraic fashion, similar to the diophantine equations used for labeling the gaps of $H^{B_0}_{\mathrm{Hof}}$. Also, the code to produce the colored butterfly of $H^{B}_{-2,3}$ in Figure 4 is taken from [Amr 2015] and based on a code originally developed by Daniel Osadchy. This algorithm, the details on the numerics, and a much more detailed study of the operator $H^{B}_{\theta,q}$ will be presented elsewhere [Amr et al. 2015]. There, we also show how to explicitly incorporate a better approximation to the true dispersion relation of a magnetic subband and the subprincipal symbol, as given in Theorem 5.1, into the Peierls substitution Hamiltonian. Then the agreement in terms of Chern numbers depicted in Figure 4 turns into a quantitative agreement also of the spectrum. We take these numerical results as an indication that Theorem 5.1 also holds for perturbations by small constant magnetic fields.

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References

[Amr 2015] A. Amr, *Chern numbers in solid state physics*, Diploma thesis, Universität Tübingen, 2015.

[Amr et al. 2015] A. Amr, G. De Nittis, and S. Teufel, "Twisted Hofstadter Hamiltonians", in preparation, 2015.

[Asch et al. 1994] J. Asch, H. Over, and R. Seiler, "Magnetic Bloch analysis and Bochner Laplacians", *J. Geom. Phys.* **13**:3 (1994), 275–288. MR 1269244 Zbl 0804.58022

[Avila and Jitomirskaya 2009] A. Avila and S. Jitomirskaya, "The ten martini problem", *Ann. of Math.* (2) **170**:1 (2009), 303–342. MR 2521117 Zbl 1166.47031

[Bellissard 1988] J. Bellissard, "C^* algebras in solid state physics: 2D electrons in a uniform magnetic field", pp. 49–76 in *Operator algebras and applications, II*, edited by D. E. Evans and M. Takesaki, London Math. Soc. Lecture Note Ser. **136**, Cambridge Univ. Press, 1988. MR 996451 Zbl 0677.46055

[Bellissard et al. 1991] J. Bellissard, C. Kreft, and R. Seiler, "Analysis of the spectrum of a particle on a triangular lattice with two magnetic fluxes by algebraic and numerical methods", *J. Phys. A* **24**:10 (1991), 2329–2353. MR 1118535 Zbl 0738.35047

[Bellissard et al. 1994] J. Bellissard, A. van Elst, and H. Schulz-Baldes, "The noncommutative geometry of the quantum Hall effect", *J. Math. Phys.* **35**:10 (1994), 5373–5451. MR 1295473 Zbl 0824.46086

[Blount 1962] E. I. Blount, "Formalisms of band theory", pp. 305–373 in *Solid state physics, XIII*, Academic Press, New York, 1962. MR 0138464

[Buslaev 1987] V. S. Buslaev, "Semiclassical approximation for equations with periodic coefficients", *Uspekhi Mat. Nauk* **42**:6 (1987), 77–98. In Russian; translated in *Russ. Math. Surveys* **42**:6 (1987), 97–125. MR 933996 Zbl 0698.35130

[De Nittis 2010] G. De Nittis, *Hunting colored (quantum) butterflies: a geometric derivation of the TKNN-equations*, Ph.D. thesis, Scuola Internazionale Superiore di Studi Avanzati, 2010, https://tel.archives-ouvertes.fr/tel-00674271/document.

[De Nittis and Lein 2011] G. De Nittis and M. Lein, "Applications of magnetic ΨDO techniques to SAPT", *Rev. Math. Phys.* **23**:3 (2011), 233–260. MR 2793476 Zbl 1214.81093

[De Nittis and Panati 2010] G. De Nittis and G. Panati, "Effective models for conductance in magnetic fields: derivation of Harper and Hofstadter models", preprint, 2010. arXiv 1007.4786

[Dimassi and Sjöstrand 1999] M. Dimassi and J. Sjöstrand, *Spectral asymptotics in the semi-classical limit*, London Mathematical Society Lecture Note Series **268**, Cambridge University Press, 1999. MR 1735654 Zbl 0926.35002

[Dimassi et al. 2004] M. Dimassi, J.-C. Guillot, and J. Ralston, "On effective Hamiltonians for adiabatic perturbations of magnetic Schrödinger operators", *Asymptot. Anal.* **40**:2 (2004), 137–146. MR 2104132 Zbl 1130.81344

[Dubrovin and Novikov 1980a] B. A. Dubrovin and S. P. Novikov, "Ground states in a periodic field: magnetic Bloch functions and vector bundles", *Dokl. Akad. Nauk SSSR* **253**:6 (1980), 1293–1297. In Russian; translated in *Soviet Math. Dokl.* **22** (1980), 240–244. MR 583789 Zbl 0489.46055

[Dubrovin and Novikov 1980b] B. A. Dubrovin and S. P. Novikov, "Ground states of a two-dimensional electron in a periodic magnetic field", *Zh. Eksper. Teoret. Fiz.* **79**:3 (1980), 1006–1016. In Russian; translated in *Soviet Physics JETP* **52** (1980), 511–516. MR 617904

[Freund 2013] S. Freund, *Effective Hamiltonians for magnetic Bloch bands*, Ph.D. thesis, Universität Tübingen, 2013, https://bibliographie.uni-tuebingen.de/xmlui/handle/10900/37930.

[Gat and Avron 2003a] O. Gat and J. E. Avron, "Magnetic fingerprints of fractal spectra and duality of Hofstadter models", *New J. Phys.* **5** (2003), 44.1–44.8.

[Gat and Avron 2003b] O. Gat and J. E. Avron, "Semiclassical analysis and the magnetization of the Hofstadter model", *Physical Review Letters* **91**:18 (2003), art. ID 186801.

[Gérard and Nier 1998] C. Gérard and F. Nier, "Scattering theory for the perturbations of periodic Schrödinger operators", *J. Math. Kyoto Univ.* **38**:4 (1998), 595–634. MR 1669979 Zbl 0934.35111

[Gérard et al. 1991] C. Gérard, A. Martinez, and J. Sjöstrand, "A mathematical approach to the effective Hamiltonian in perturbed periodic problems", *Comm. Math. Phys.* **142**:2 (1991), 217–244. MR 1137062 Zbl 0753.35057

[Guillot et al. 1988] J.-C. Guillot, J. Ralston, and E. Trubowitz, "Semiclassical asymptotics in solid state physics", *Comm. Math. Phys.* **116**:3 (1988), 401–415. MR 937768 Zbl 0672.35014

[Hansen 2011] S. Hansen, "Rayleigh-type surface quasimodes in general linear elasticity", *Anal. PDE* **4**:3 (2011), 461–497. MR 2872123 Zbl 1264.35248

[Helffer and Sjöstrand 1989] B. Helffer and J. Sjöstrand, "Équation de Schrödinger avec champ magnétique et équation de Harper", pp. 118–197 in *Schrödinger operators* (Sønderborg, 1988), edited by H. Holden and A. Jensen, Lecture Notes in Phys. **345**, Springer, Berlin, 1989. MR 1037319 Zbl 0699.35189

[Helffer and Sjöstrand 1990a] B. Helffer and J. Sjöstrand, *Analyse semi-classique pour l'équation de Harper, II: Comportement semi-classique près d'un rationnel*, Mém. Soc. Math. France (N.S.) **40**, Société Mathématique de France, Paris, 1990. MR 1052373 Zbl 0714.34131

[Helffer and Sjöstrand 1990b] B. Helffer and J. Sjöstrand, "On diamagnetism and de Haas-van Alphen effect", *Ann. Inst. H. Poincaré Phys. Théor.* **52**:4 (1990), 303–375. MR 1062904 Zbl 0715.35070

[Helffer et al. 1990] B. Helffer, P. Kerdelhué, and J. Sjöstrand, *Le papillon de Hofstadter revisité*, Mém. Soc. Math. France (N.S.) **43**, Société Mathématique de France, Paris, 1990. MR 1090467 Zbl 0732.44004

[Hofstadter 1976] D. R. Hofstadter, "Energy levels and wave functions of Bloch electrons in rational and irrational magnetic fields", *Phys. Rev. B* **14**:6 (1976), 2239–2249.

[Hörmander 1985] L. Hörmander, *The analysis of linear partial differential operators, IV: Pseudodifferential operators*, Grundlehren der Math. Wissenschaften **274**, Springer, Berlin, 1985. MR 781537 Zbl 0601.35001

[Hövermann et al. 2001] F. Hövermann, H. Spohn, and S. Teufel, "Semiclassical limit for the Schrödinger equation with a short scale periodic potential", *Comm. Math. Phys.* **215**:3 (2001), 609–629. MR 1810947 Zbl 1052.81039

[Martinez and Sordoni 2002] A. Martinez and V. Sordoni, "A general reduction scheme for the time-dependent Born–Oppenheimer approximation", *C. R. Math. Acad. Sci. Paris* **334**:3 (2002), 185–188. MR 1891055 Zbl 1079.81524

[Nenciu 1991] G. Nenciu, "Dynamics of band electrons in electric and magnetic fields: rigorous justification of the effective Hamiltonians", *Reviews of Modern Physics* **63** (1991), 91–128.

[Nenciu 2002] G. Nenciu, "On asymptotic perturbation theory for quantum mechanics: almost invariant subspaces and gauge invariant magnetic perturbation theory", *J. Math. Phys.* **43**:3 (2002), 1273–1298. MR 1885006 Zbl 1059.81064

[Nenciu and Sordoni 2004] G. Nenciu and V. Sordoni, "Semiclassical limit for multistate Klein–Gordon systems: almost invariant subspaces, and scattering theory", *J. Math. Phys.* **45**:9 (2004), 3676–3696. MR 2081813 Zbl 1071.81043

[Novikov 1981] S. P. Novikov, "Magnetic Bloch functions and vector bundles: typical dispersion laws and their quantum numbers", *Dokl. Akad. Nauk SSSR* **257**:3 (1981), 538–543. In Russian; translated in *Soviet Math. Dokl.* **23** (1981), 298–303. Zbl 0483.46054

[Osadchy and Avron 2001] D. Osadchy and J. E. Avron, "Hofstadter butterfly as quantum phase diagram", *J. Math. Phys.* **42**:12 (2001), 5665–5671. MR 1866679 Zbl 1019.81071

[Panati 2007] G. Panati, "Triviality of Bloch and Bloch–Dirac bundles", *Ann. Henri Poincaré* **8**:5 (2007), 995–1011. MR 2342883 Zbl 05207467

[Panati et al. 2003a] G. Panati, H. Spohn, and S. Teufel, "Effective dynamics for Bloch electrons: Peierls substitution and beyond", *Comm. Math. Phys.* **242**:3 (2003), 547–578. MR 2020280 Zbl 1058.81020

[Panati et al. 2003b] G. Panati, H. Spohn, and S. Teufel, "Space-adiabatic perturbation theory", *Adv. Theor. Math. Phys.* **7**:1 (2003), 145–204. MR 2014961

[Peierls 1933] R. Peierls, "Zur Theorie des Diamagnetismus von Leitungselektronen", *Zeitschrift fur Physik* **80**:11–12 (1933), 763–791. Zbl 0006.19204

[Pflaum 1998a] M. J. Pflaum, "A deformation-theoretical approach to Weyl quantization on Riemannian manifolds", *Lett. Math. Phys.* **45**:4 (1998), 277–294. MR 1653420 Zbl 0995.53057

[Pflaum 1998b] M. J. Pflaum, "The normal symbol on Riemannian manifolds", *New York J. Math.* **4** (1998), 97–125. MR 1640055 Zbl 0903.35099

[Rammal and Bellissard 1990] R. Rammal and J. Bellissard, "An algebraic semi-classical approach to Bloch electrons in a magnetic field", *Journal de Physique* **51** (1990), 1803–1830.

[Safarov 1997] Y. Safarov, "Pseudodifferential operators and linear connections", *Proc. London Math. Soc.* (3) **74**:2 (1997), 379–416. MR 1425328 Zbl 0872.35140

[Schulz-Baldes and Teufel 2013] H. Schulz-Baldes and S. Teufel, "Orbital polarization and magnetization for independent particles in disordered media", *Comm. Math. Phys.* **319**:3 (2013), 649–681. MR 3040371 Zbl 1271.82022

[Sharafutdinov 2004] V. A. Sharafutdinov, "A geometric symbolic calculus for pseudodifferential operators, I", *Mat. Tr.* **7**:2 (2004), 159–206. In Russian; translated in *Siberian Adv. Math.* **15** (2005), 81–125. MR 2124544 Zbl 1081.58016

[Sharafutdinov 2005] V. A. Sharafutdinov, "A geometric symbolic calculus for pseudodifferential operators, II", *Mat. Tr.* **8**:1 (2005), 176–201. In Russian; translated in *Siberian Adv. Math.* **15** (2005), 71–95. MR 1955026 Zbl 1082.58025

[Stiepan 2011] H.-M. Stiepan, *Adiabatic perturbation theory for magnetic Bloch Bands*, Ph.D. thesis, Universität Tübingen, 2011.

[Stiepan and Teufel 2013] H.-M. Stiepan and S. Teufel, "Semiclassical approximations for Hamiltonians with operator-valued symbols", *Comm. Math. Phys.* **320**:3 (2013), 821–849. MR 3057191 Zbl 1268.81079

[Sundaram and Niu 1999] G. Sundaram and Q. Niu, "Wave-packet dynamics in slowly perturbed crystals: gradient corrections and Berry-phase effects", *Phys. Rev. B* **59**:23 (1999), 14915–14925.

[Teufel 2003] S. Teufel, *Adiabatic perturbation theory in quantum dynamics*, Lecture Notes in Mathematics **1821**, Springer, Berlin, 2003. MR 2158392 Zbl 1053.81003

[Teufel 2012] S. Teufel, "Semiclassical approximations for adiabatic slow-fast systems", *Europhysics Letters* **98**:5 (2012), art. ID 50003.

[Thouless et al. 1982] D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, "Quantized Hall conductance in a two-dimensional periodic potential", *Phys. Review Letters* **49**:6 (1982), 405–408.

[Widom 1978] H. Widom, "Families of pseudodifferential operators", pp. 345–395 in *Topics in functional analysis (essays dedicated to M. G. Kreĭn on the occasion of his* 70*-th birthday)*, edited by I. Gohberg and M. Kac, Adv. in Math. Suppl. Stud. **3**, Academic Press, New York, 1978. MR 538027 Zbl 0477.58035

[Widom 1980] H. Widom, "A complete symbolic calculus for pseudodifferential operators", *Bull. Sci. Math.* (2) **104**:1 (1980), 19–63. MR 560744 Zbl 0434.35092

[Xiao et al. 2010] D. Xiao, M.-C. Chang, and Q. Niu, "Berry phase effects on electronic properties", *Rev. Modern Phys.* **82**:3 (2010), 1959–2007. MR 2734353 Zbl 1243.82059

[Zak 1968] J. Zak, "Dynamics of Electrons in Solids in External Fields", *Phys. Review* **168**:3 (1968), 686–695.

[Zak 1986] J. Zak, "Effective hamiltonians and magnetic energy bands?", *Phys. Letters A* **117**:7 (1986), 367–371.

[Zak 1991] J. Zak, "Exact symmetry of approximate effective Hamiltonians", *Phys. Rev. Letters* **67** (1991), 2565–2568.

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DISPERSIVE ESTIMATES IN $\mathbb{R}^3$ WITH THRESHOLD EIGENSTATES AND RESONANCES

MARIUS BECEANU

We prove dispersive estimates in $\mathbb{R}^3$ for the Schrödinger evolution generated by the Hamiltonian $H = -\Delta + V$, under optimal decay conditions on V, in the presence of zero-energy eigenstates and resonances.

1. Introduction

1A. *Classification of exceptional Hamiltonians.* Consider a Hamiltonian of the form $H = -\Delta + V$, where V is a real-valued scalar potential on $\mathbb{R}^3$.

We assume $V \in L^{\frac{3}{2},1} \subset L^{\frac{3}{2}}$, which is the predual of weak-L^3 and a Lorentz space, $L^{\frac{3}{2},1} \subset L^{\frac{3}{2}-\epsilon} \cap L^{\frac{3}{2}+\epsilon}$; for its definition and properties, see [Bergh and Löfström 1976]. By [Simon 1982], this is sufficient to guarantee the self-adjointness of $H = -\Delta + V$.

Let $R_0(\lambda) := (-\Delta - \lambda)^{-1}$ be the free resolvent corresponding to the free evolution $e^{-it\Delta}$ and let $R_V(\lambda) := (-\Delta + V - \lambda)^{-1}$ be the perturbed resolvent corresponding to the perturbed evolution e^{itH}. Explicitly, in three dimensions and for $\operatorname{Im} \lambda \geq 0$,

$$R_0((\lambda + i0)^2)(x, y) = \frac{1}{4\pi} \frac{e^{i\lambda|x-y|}}{|x-y|}. \tag{1-1}$$

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It will be shown below that, under reasonable assumptions, H has only finitely many negative eigenvalues. Then the Schrödinger evolution restricted to the continuous spectrum $[0,\infty)$ has the representation formula

$$e^{itH}P_c = \lim_{\epsilon\to 0}\frac{1}{2\pi i}\int_0^\infty e^{it\eta}\big(R_V(\eta+i\epsilon)-R_V(\eta-i\epsilon)\big)\,d\eta.$$

By the work of Ionescu and Jerison [2003] and Goldberg and Schlag [2004b], it is known that, when $V\in L^{\frac{3}{2}}$, the perturbed resolvent $R_V(\lambda\pm i0)$ is uniformly bounded in $\mathcal{B}(L^{\frac{6}{5}},L^6)$ on any interval $\lambda\in[\epsilon_0,\infty)$, where $\epsilon_0>0$, and has no singularities in $[0,\infty)$ except potentially at $\lambda=0$.

Observe that $R_V=(I+R_0V)^{-1}R_0$, so R_V has a singularity at zero precisely when $I+R_0(0)V$, which is a compact perturbation of the identity, is not invertible.

We denote the null space of $I+R_0(0)V$ by

$$\mathcal{M}:=\big\{\phi\in L^\infty \mid \phi+R_0(0)V\phi=0\big\}.$$

If $\mathcal{M}\neq\varnothing$, we say that H is of *exceptional type*, while if $\mathcal{M}=\varnothing$, we say that H is of *generic type*.

The sesquilinear form $-\langle u,Vv\rangle$ is an inner product on $\mathcal{M}$; see Lemma 2.2. This pairing is well-defined when $V\in L^{\frac{3}{2},1}$ because $u,v\in L^{3,\infty}\cap L^\infty$ by Lemma 2.1.

Let $\mathcal{E}:=\mathcal{M}\cap L^2$ and P_0 be the orthogonal L^2 projection onto $\mathcal{E}$. In Lemma 2.3, we provide a characterization of $\mathcal{E}$ and show that $\operatorname{codim}_{\mathcal{M}}\mathcal{E}\le 1$.

The set $\mathcal{E}_1:=\mathcal{E}\cap L^1$ also plays a special part in the proof. In Lemma 2.5, we give a characterization of $\mathcal{E}_1$ and prove that $\operatorname{codim}_{\mathcal{E}}\mathcal{E}_1\le 12$.

A function $\phi\in\mathcal{M}\setminus\mathcal{E}$ is called a zero-energy resonance of H. Following [Jensen and Kato 1979; Yajima 2005], we classify exceptional Hamiltonians H as follows:

(1) H is of exceptional type of the first kind if it has a zero-energy resonance, but no zero-energy eigenfunctions: $\{0\}=\mathcal{E}\subsetneq\mathcal{M}$.

(2) H is of exceptional type of the second kind if it has zero-energy eigenfunctions, but no zero-energy resonance: $\{0\}\subsetneq\mathcal{E}=\mathcal{M}$.

(3) H is of exceptional type of the third kind if it has both resonances and eigenfunctions at zero energy: $\{0\}\subsetneq\mathcal{E}\subsetneq\mathcal{M}$.

1B. *Main result.* When H is of exceptional type of the first kind, we let the *canonical resonance* be $\phi\in\mathcal{M}$ such that $\langle V,\phi\rangle>0$ and $-\langle\phi,V\phi\rangle=1$ (one can make these choices by Lemmas 2.3 and 2.2, respectively).

Using the canonical resonance $\phi(x)$, we define a constant a and a function $\zeta_t(x)$ by

$$a=\frac{4\pi i}{|\langle V,\phi\rangle|^2},\qquad \zeta_t(x)=e^{\frac{i|x|^2}{4t}}\phi(x).$$

We also define a function $\mu_t(x)$ by

$$\mu_t(x):=\frac{i}{|x|}\int_0^1\big(e^{\frac{i|x|^2}{4t}}-e^{\frac{i|\theta x|^2}{4t}}\big)\,d\theta.$$

Let the operators $R(t)$ and $S(t)$ be given by

$$\begin{aligned} R(t) &:= \frac{ae^{-i\frac{3\pi}{4}}}{\sqrt{\pi t}}\zeta_t(x)\otimes\zeta_t(y), \\ S(t) &:= \frac{e^{-i\frac{3\pi}{4}}}{\sqrt{\pi t}}\biggl(-iP_0V\frac{|x-y|^2}{24\pi}VP_0+\mu_t(x)\frac{|x-y|}{8\pi}VP_0+P_0V\frac{|x-y|}{8\pi}\mu_t(y)\biggr). \end{aligned} \tag{1-2}$$

Note that

$$\|R(t)u\|_{L^{3,\infty}}+\|S(t)u\|_{L^{3,\infty}}\lesssim t^{-\frac{1}{2}}\|u\|_{L^{3/2,1}}.$$

Proposition 1.1 (main result). *Assume that* $\langle x\rangle^2V\in L^{\frac{3}{2},1}$ *and that* $H=-\Delta+V$ *is exceptional of the first kind. Then, for* $1\le p<\frac{3}{2}$ *and any* $u\in L^2\cap L^p$,

$$e^{-itH}P_cu=Z(t)u+R(t)u,\quad \|Z(t)u\|_{L^{p'}}\lesssim t^{-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{p'}\right)}\|f\|_{L^p},$$

where p' *is the dual exponent, that is,* $\frac{1}{p}+\frac{1}{p'}=1$. *Furthermore, assuming only that* $V\in L^{\frac{3}{2},1}$, *for* $\frac{3}{2}<p\le 2$,

$$\|e^{-itH}P_cu\|_{L^{p'}}\lesssim t^{-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{p'}\right)}\|u\|_{L^p},\quad \|e^{-itH}P_cu\|_{L^{3,\infty}}\lesssim t^{-\frac{1}{2}}\|u\|_{L^{3/2,1}}.$$

Assume that $\langle x\rangle^4V\in L^{\frac{3}{2},1}$ *and that* $H=-\Delta+V$ *is exceptional of the second or third kind. Then, for* $1\le p<\frac{3}{2}$ *and any* $u\in L^2\cap L^p$,

$$e^{-itH}P_cu=Z(t)u+R(t)u+S(t)u,\quad \|Z(t)u\|_{L^{p'}}\lesssim t^{-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{p'}\right)}\|u\|_{L^p}, \tag{1-3}$$

where $R(t)$ *is missing if* H *is an exceptional Hamiltonian of the second kind.*

In the case when all the zero-energy eigenfunctions of H *are in* L^1, *one can omit* $S(t)$ *from* (1-3).

Assume that $\langle x\rangle^2V\in L^{\frac{3}{2},1}$ *and that* $H=-\Delta+V$ *is exceptional of the second or third kind. Then, for* $\frac{3}{2}<p\le 2$,

$$\|e^{-itH}P_cu\|_{L^{p'}}\lesssim t^{-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{p'}\right)}\|u\|_{L^p},\quad \|e^{-itH}P_cu\|_{L^{3,\infty}}\lesssim t^{-\frac{1}{2}}\|u\|_{L^{3/2,1}}.$$

Note that, in terms of powers of x, the decay conditions on the potential correspond to $|V|\lesssim\langle x\rangle^{-2-}$, $|V|\lesssim\langle x\rangle^{-4-}$, and $|V|\lesssim\langle x\rangle^{-6-}$.

Additionally, note that these decay estimates also imply a certain range of Strichartz estimates.

The rest of the paper is dedicated to proving this main result, which is a combination of Propositions 2.13, 2.15, 2.18, and 2.19. For brevity, we omit the proof in the case when H is an exceptional Hamiltonian of the second kind, which is similar to the case when H is exceptional of the third kind.

1C. ***History of the problem.*** We study solutions to the linear Schrödinger equation in $\mathbb{R}^3$ with potential

$$i\partial_tu+\Delta u-Vu=0,\quad u(0)\text{ given.}$$

By the RAGE theorem, every solution is the sum of a bound and a scattering component. The quantitative study of scattering states began with Rauch [1978], who proved that if $H=-\Delta+gV$, where $g\in\mathbb{C}$, with exponentially decaying V, then $e^{itH} P_c$ has a local decay rate of $t^{-\frac{3}{2}}$, with at most a discrete set of exceptional g for which the decay rate is $t^{-\frac{1}{2}}$. Here P_c is the projection on the space of scattering solutions.

Threshold estimates in the presence of eigenvalues and resonances go back to the work of Jensen and Kato [1979], who obtained an asymptotic expansion of the resolvent $R(\zeta) = (H - \zeta)^{-1}$ into

$$R(\zeta) = -\zeta^{-1} B_{-2} - i\zeta^{-\frac{1}{2}} B_{-1} + B_0 + i\zeta^{\frac{1}{2}} B_1 + \cdots$$

and similar ones for the spectral density and the S-matrix. The condition imposed on the potential was polynomial decay at infinity of the form $(1 + |x|^{\beta})V(x) \in L^{\frac{3}{2}}(\mathbb{R}^3)$, where $\beta > 2$.

The possible singularities in this expansion are due to the presence of resonances or eigenstates at zero. B_{-2} is the L^2 orthogonal projection on the zero eigenspace, while B_{-1} is given by

$$B_{-1} = P_0 V \frac{|x-y|^2}{24\pi} V P_0 - \phi \otimes \phi,$$

where ϕ is the canonical zero resonance; see above.

Jensen and Kato also obtained an asymptotic expansion for the evolution $e^{itH} P_c$ in two cases: if zero is a regular point, then

$$e^{itH} P_c = -(4\pi i)^{-\frac{1}{2}} t^{-\frac{3}{2}} B_0 + o(t^{-\frac{3}{2}}),$$

and if there is only a resonance ϕ at zero then

$$e^{itH} P_c = (\pi i)^{-\frac{1}{2}} t^{-\frac{1}{2}} \phi \otimes \phi + o(t^{-\frac{1}{2}}).$$

Murata [1982] extended these results by obtaining an asymptotic expansion to any order, for a more general evolution, with or without singular points, and then proving that each term in the expansion is degenerate. Murata's expansion and proof are valid in weighted L^2 spaces.

Erdoğan and Schlag [2004] obtained an asymptotic expansion of the evolution $e^{itH} P_c$ in the pointwise L^1-to-L^∞ setting using the Jensen–Nenciu lemma [2001]. The condition assumed for the potential was that $|V(x)| \lesssim \langle x \rangle^{-12-\epsilon}$. The same method works in the case of nonselfadjoint Hamiltonians (see [Erdoğan and Schlag 2006]) of the form

$$\mathcal{H} = \begin{pmatrix} -\Delta+\mu+V_1 & V_2 \\ -V_2 & \Delta-\mu-V_1 \end{pmatrix},$$

assuming that $|V_1(x)| + |V_2(x)| \lesssim \langle x \rangle^{-10-\epsilon}$.

At the same time, Yajima [2005] proved a similar expansion for generic Hamiltonians $H = -\Delta + V$ when $|V(x)| \le \langle x \rangle^{-\frac{5}{2}-\epsilon}$, for singular Hamiltonians of the first kind when $|V(x)| \le \langle x \rangle^{-\frac{9}{2}-\epsilon}$, and of the second and third kind when $|V(x)| \le \langle x \rangle^{-\frac{11}{2}-\epsilon}$. His main result stated the following:

Theorem 1.2 [Yajima 2005, Theorem 1.3]. (1) *Let V satisfy $|V(x)| \le C\langle x \rangle^{-\beta}$ for some $\beta > \frac{5}{2}$. Suppose that H is of generic type. Then, for any $1 \le q \le 2 \le p \le \infty$ such that $\frac{1}{p} + \frac{1}{q} = 1$,*

$$\|e^{-itH} P_c u\|_p \le C_p t^{-3\left(\frac{1}{2}-\frac{1}{p}\right)} \|u\|_q, \quad \text{where } u \in L^2 \cap L^q. \tag{1-4}$$

(2) *Let V satisfy $|V(x)| \leq C\langle x\rangle^{-\beta}$ for some $\beta > \frac{11}{2}$. Suppose that H is of exceptional type. Then the following statements are satisfied*:

(a) *Estimate* (1-4) *holds when p and q are restricted to $\frac{3}{2} < q \leq 2 \leq p < 3$ and $\frac{1}{p} + \frac{1}{q} = 1$.*

(b) *Estimate* (1-4) *holds when $p = 3$ and $q = \frac{3}{2}$ provided that L^3 and $L^{\frac{3}{2}}$ are respectively replaced by Lorentz spaces $L^{3,\infty}$ and $L^{\frac{3}{2},1}$.*

(c) *When $3 < p \leq \infty$ and $1 \leq q < \frac{3}{2}$ are such that $\frac{1}{p} + \frac{1}{q} = 1$, there exists a constant C_{pq} such that, for any $u \in L^2 \cap L^q$,*

$$\left\|(e^{-itH} P_c - R(t) - S(t))u\right\|_p \lesssim C_{pq} t^{-3\left(\frac{1}{2}-\frac{1}{p}\right)} \|u\|_q.$$

If H is of exceptional type of the first kind, statement (2) *holds under a weaker decay condition $|V(x)| \leq C\langle x\rangle^{-\beta}$ with $\beta > \frac{9}{2}$.*

However, note that, due to a mistake in the proof, the requirement $\beta > \frac{11}{2}$ should be replaced by $\beta > 8$.

When the zero-energy eigenfunctions ϕ_k of H have enough decay, both $R(t)$ and $S(t)$ can be taken to be zero. Indeed, Goldberg [2010] showed that if $V \in L^{\frac{3}{2}-\epsilon} \cap L^{\frac{3}{2}+\epsilon}$ and the zero-energy eigenfunctions are in L^1 then $\|e^{-itH} P_c u\|_{L^\infty} \lesssim t^{-\frac{3}{2}} \|u\|_{L^1}$. We retrieve a similar result in our context.

Some of our results for exceptional potentials of the first kind hold under the same decay assumption as those for generic potentials: $V \in L^{\frac{3}{2},1}$. A similar fact was also recently noticed by Egorova, Kopylova, Marchenko and Teschl [Egorova et al. 2014] in dimension one.

Several results [Journé et al. 1991; Goldberg and Schlag 2004a; Goldberg 2006; Beceanu and Goldberg 2012] address the issue of pointwise decay in the case of generic Hamiltonians — for $L^{\frac{3}{2}-\epsilon} \cap L^{\frac{3}{2}+\epsilon}$ potentials in [Goldberg 2006] and Kato-class potentials in [Beceanu and Goldberg 2012].

Results obtained in other dimensions include [Cardoso et al. 2009; Egorova et al. 2014; Erdoğan et al. 2014; Erdoğan and Green 2010; 2013a; 2013b; 2013c; Goldberg 2007; Goldberg and Green 2014; 2015; Green 2012; Schlag 2005].

The current result, Proposition 1.1, represents an improvement on [Yajima 2005] by half a power of potential decay for exceptional Hamiltonians of the first kind. We expect the rate of potential decay from Proposition 1.1 to be optimal for this sort of result.

The same considerations apply in the case of exceptional Hamiltonians of the second and third kind, also leading to similar improved results. These will constitute the subject of a separate paper.

Below we mostly follow the scheme of Yajima's proof [2005], making the changes from Hölder spaces to Wiener spaces needed to improve the result. The proof method that we use here is the same as in [Beceanu 2011; Beceanu and Goldberg 2012].

2. Proof of the statements

2A. ***Notations.*** We denote the usual Lebesgue spaces by L^p and the Lorentz spaces by $L^{p,q}$, where $1 \leq p, q \leq \infty$. Note here that $L^{p,p} = L^p$, $L^{p,\infty}$ is weak-L^p, and $L^{p,q_1} \subset L^{p,q_2}$ for $q_1 \leq q_2$. For the definition and further properties, see [Bergh and Löfström 1976].

Let Sobolev spaces be $W^{s,p}$, where $s \in \mathbb{R}$ and $1 \le p \le \infty$, and denote weighted Lebesgue spaces by $f(x)L^p = \{f(x)g(x) \mid g \in L^p\}$.

Fix the Fourier transform to

$$\hat{f}(\xi) = \int_{\mathbb{R}^d} e^{-ix\xi} f(x)\,dx, \quad \check{f}(x) = (2\pi)^{-d} \int_{\mathbb{R}^d} e^{i\xi x} f(\xi)\,d\xi.$$

Let $R_0(\lambda) := (-\Delta - \lambda)^{-1}$ and for $\lambda \in \mathbb{R}$,

$$R_{0a}(\lambda) := \frac{1}{i}\big(R_0(\lambda + i0) - R_0(\lambda - i0)\big).$$

Concerning the Fourier transform, resolvents, and the free evolution, note that with our definitions

$$\begin{aligned} e^{itH_0} &= (R_{0a}(\lambda))^{\vee}(t), \\ R_{0a}(\lambda) &= (e^{itH_0})^{\wedge} \quad \text{for } \lambda \in \mathbb{R}, \\ iR_0(\lambda) &= \big(\chi_{[0,\infty)}(t) e^{itH_0}\big)^{\wedge}(\lambda) \quad \text{for } \operatorname{Im} \lambda < 0. \end{aligned}$$

Likewise let $R_V(\lambda) := (-\Delta + V - \lambda)^{-1}$.

Also, let

- χ_A be the characteristic function of the set A;
- $\mathcal{M}$ be the space of finite-mass Borel measures on $\mathbb{R}$;
- δ_x denote Dirac's measure at x;
- $\langle x \rangle = (1 + |x|^2)^{\frac{1}{2}}$;
- $\mathcal{B}(X, Y)$ be the Banach space of bounded operators from X to Y and $\mathcal{B}(X)$ be the Banach space of bounded operators from X to itself;
- C be any constant (not always the same throughout the paper);
- $a \lesssim b$ mean $|a| \le C|b|$;
- $\mathcal{S}$ be the Schwartz space;
- $u \otimes v$ mean the rank-one operator $\langle \cdot, v \rangle u$;
- $K(x, y)$ denote the operator having $K(x, y)$ as its integral kernel.

For a potential V, let $V_1 = |V|^{\frac{1}{2}}$ and $V_2 = |V|^{\frac{1}{2}} \operatorname{sgn} V$.

2B. ***Auxiliary results.*** Recall that $\mathcal{M}$ is the kernel of $I + R_0(0)V$ in L^∞.

Lemma 2.1. *Let $V \in L^{\frac{3}{2},1}$; then $\mathcal{M} \subset L^{3,\infty}$. Conversely, any $\phi \in L^{3,\infty}$ that satisfies the equation $\phi + R_0(0)V\phi = 0$ must be in L^∞, hence in $\mathcal{M}$.*

Proof of Lemma 2.1. Let $V = V^1 + V^2$, where V^1 is smooth of compact support and $\|V^2\|_{L^{3/2,1}} \ll 1$. Then, if ϕ solves the equation

$$\begin{aligned} \phi &= -\big(I + R_0(0)V^2\big)^{-1} R_0(0)V^1\phi \\ &= -\Big(\sum_{k=0}^{\infty} (-1)^k (R_0(0)V^2)^k\Big) R_0(0)V^1\phi, \end{aligned}$$

where the inverse is the sum of a Neumann series, and thus is bounded on $L^{3,\infty}$ and on L^∞.

If $\phi \in L^\infty$, then $V^1\phi \in L^1$; hence $R_0(0)V^1\phi \in L^{3,\infty}$, so $\phi \in L^{3,\infty}$.

If $\phi \in L^{3,\infty}$, then $V^1\phi \in L^{\frac{3}{2},1}$; hence $R_0(0)V^1\phi \in L^\infty$, so $\phi \in L^\infty$. □

Lemma 2.2. *The quadratic form $-\langle u, Vv\rangle$ is an inner product on $\mathcal{M}$.*

Proof. Suppose that $u, v \in \mathcal{M}$. By the definition of $\mathcal{M}$, observe that $-\langle u, Vv\rangle = \langle u, -\Delta v\rangle$, where $u \in L^{3,\infty} \cap L^\infty$ by Lemma 2.1 and $-\Delta v = Vv \in L^1 \cap L^{\frac{3}{2},1}$. Thus the pairing is well-defined.

Furthermore, $\nabla u = \nabla R_0(0)Vu \in L^{\frac{3}{2},\infty} \cap L^{3,\infty} \subset L^2$ and the same holds for ∇v, so their pairing is also well-defined and we can write $(u, -\Delta v) = (\nabla u, \nabla v)$.

This expression is positively defined because, setting $u = v$, the equation $\langle \nabla u, \nabla u\rangle = 0$ implies that u is constant; hence, in view of the fact that $u \in L^{3,\infty}$ by Lemma 2.1, $u = 0$. □

Recall that $\mathcal{E} = \mathcal{M} \cap L^2$.

Lemma 2.3. *Assume that $V \in L^{\frac{3}{2},1}$. Then, for any $\phi \in \mathcal{M}$, we have $\phi(x) \in \langle x\rangle^{-1}L^\infty$.*

Assume that $V \in L^1 \cap L^{\frac{3}{2},1}$. Then, for any $\phi \in \mathcal{M}$, we have

$$\phi(x) - \frac{\langle \phi, V\rangle}{4\pi|x|} \in |x|^{-1}L^{3,\infty} \cap |x|^{-1}L^\infty \subset L^2.$$

Thus $\phi \in \mathcal{M}$ is in $\mathcal{E}$ if and only if $\langle \phi, V\rangle = 0$; thus $\operatorname{codim}_{\mathcal{M}} \mathcal{E} \le 1$. *Also, $\mathcal{E} \subset \langle x\rangle^{-2}L^\infty$.*

Proof of Lemma 2.3. First, assume that $V \in L^{\frac{3}{2},1}$. Rewrite the eigenfunction equation

$$\phi(x) = -\frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{1}{|x-y|} V(y)\phi(y)\,dy$$

as

$$|x|\phi(x) + \frac{1}{4\pi}\int_{|y|\ge R} \frac{|x|-|x-y|}{|x-y|\,|y|} V(y)|y|\phi(y)\,dy$$
$$= -\frac{1}{4\pi}\int_{\mathbb{R}^3} V(y)\phi(y)\,dy - \frac{1}{4\pi}\int_{|y|\le R} \frac{|x|-|x-y|}{|x-y|} V(y)\phi(y)\,dy.$$

Note that $\big||x|-|x-y|\big| \le |y|$ and $\lim_{R\to\infty} \|\chi_{|x|\ge R}(x)V(x)\|_{L^{3/2,1}} = 0$. Then, for sufficiently large R, we can invert

$$(T_0\phi)(x) = \phi(x) + \frac{1}{4\pi}\int_{|y|\ge R} \frac{|x|-|x-y|}{|x-y|\,|y|} V(y)\phi(y)\,dy$$

as an operator in $\mathcal{B}(L^\infty)$. Since $\phi(y) \in L^{3,\infty} \cap L^\infty$, the right-hand side is in L^∞, so we obtain that $|x|\phi(x) \in L^\infty$.

Next, assume that $V \in L^1 \cap L^{\frac{3}{2},1}$. Start from

$$\phi(x) - \frac{\langle \phi, V\rangle}{4\pi|x|} = -\frac{1}{4\pi}\int_{\mathbb{R}^3} \left(\frac{1}{|x-y|} - \frac{1}{|x|}\right) V(y)\phi(y)\,dy$$
$$= -\frac{1}{4\pi|x|}\int_{\mathbb{R}^3} \frac{|x|-|x-y|}{|x-y|} V(y)\phi(y)\,dy,$$

which is bounded in absolute value by

$$\frac{1}{4\pi|x|}\int_{\mathbb{R}^3} \frac{|y|\,|V(y)|\,|\phi(y)|}{|x-y|}\,dy.$$

Since $\phi \in \langle x\rangle^{-1} L^\infty$ and $V \in L^1 \cap L^{\frac{3}{2},1}$, this expression is in $|x|^{-1} L^\infty \cap |x|^{-1} L^{3,\infty} \subset \langle x\rangle^{-1} L^{3,\infty} \subset L^2$.

Since whenever $\langle \phi, V\rangle \neq 0$ we have $\langle \phi, V\rangle/(4\pi|x|) \notin L^2$, it follows that for ϕ to be in L^2 it is necessary and sufficient that $\langle \phi, V\rangle = 0$.

The space $\mathcal{E}$ is then the kernel of the rank-one map $\phi \mapsto \langle \phi, V\rangle$ from $\mathcal{M}$ to $\mathbb{C}$, so it has codimension at most 1.

Finally, we already know that $\mathcal{E} \subset \mathcal{M} \subset \langle x\rangle^{-1} L^\infty$. The eigenfunction equation for a function $\phi \in \mathcal{E}$ for which $\langle \phi, V\rangle = 0$, can be written as

$$\phi(x) = -\frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{|x| - |x-y|}{|x-y|\,|x|} V(y)\phi(y)\, dy.$$

We further rewrite it as

$$|x|^2\phi(x) + \frac{1}{4\pi} \int_{|y|\geq R} \frac{(|x|-|x-y|)^2}{|x-y|\,|y|^2} V(y)|y|^2\phi(y)\, dy \\ = -\frac{1}{4\pi}\int_{\mathbb{R}^3} (|x|-|x-y|)V(y)\phi(y)\, dy - \frac{1}{4\pi}\int_{|y|\leq R} \frac{(|x|-|x-y|)^2}{|x-y|} V(y)\phi(y)\, dy.$$

The right-hand side is in L^∞ and, for sufficiently large R, the left-hand side is invertible, as above. This shows that $|x|^2\phi(x) \in L^\infty$. □

We can continue the asymptotic expansion of eigenfunctions to any order, but first we need the following lemma.

Lemma 2.4. *For* $x, y \in \mathbb{R}^3$,

$$\left| \frac{1}{|x-y|} - \left(\frac{1}{|x|} + \frac{xy}{|x|^3} \right) \right| \lesssim \frac{|y|^2}{|x|^2|x-y|} \tag{2-1}$$

and

$$\left| \frac{1}{|x-y|} - \left(\frac{1}{|x|} + \frac{xy}{|x|^3} + \frac{|y|^2}{2|x|^3} - \frac{3(xy)^2}{2|x|^5} \right) \right| \lesssim \frac{|y|^3}{|x|^3|x-y|}. \tag{2-2}$$

More generally, it seems to be the case (one can prove by induction) that

$$\left| \frac{1}{|x+y|} - \sum_{k=0}^{N} d^k \frac{1}{|x-\cdot|}(y,\dots,y) \right| \lesssim \frac{|y|^{N+1}}{|x|^{N+1}|x-y|}.$$

Proof of Lemma 2.4. Indeed, we start from

$$(|x|^2 + 2xy + |y|^2)^{\frac{1}{2}} - (|x|^2)^{\frac{1}{2}} = \frac{2xy}{|x+y|+|x|} + \frac{|y|^2}{|x+y|+|x|}. \tag{2-3}$$

Then

$$\left| \frac{2xy}{|x+y|+|x|} - \frac{xy}{|x|} \right| = \left| \frac{xy(|x|-|x+y|)}{(|x+y|+|x|)|x|} \right| \lesssim \frac{|y|^2}{|x|}.$$

Therefore,

$$\left| |x+y| - |x| - \frac{xy}{|x|} \right| \lesssim \frac{|y|^2}{|x|}. \tag{2-4}$$

Consequently,

$$\big||x|^2(|x|-|x-y|)-xy|x-y|\big| \le |x|^2\left||x-y|-|x|+\frac{xy}{|x|}\right| + \big|xy(|x|-|x-y|)\big| \lesssim |y|^2|x|.$$

Dividing by $|x|^3|x-y|$, we obtain (2-1).

We next perform a more detailed analysis of the same inequality. In (2-3), by (2-4) we have

$$\left|\frac{xy(|x|-|x+y|)}{(|x+y|+|x|)|x|}+\frac{(xy)^2}{2|x|^3}\right| \lesssim \left|\frac{xy(|x|-|x+y|)}{(|x+y|+|x|)|x|}-\frac{xy(|x|-|x+y|)}{2|x|^2}\right| + \left|\frac{xy\big(\frac{xy}{|x|}+|x|-|x+y|\big)}{2|x|^2}\right| \lesssim \frac{|y|^3}{|x|^2}.$$

Furthermore, also in (2-3),

$$\frac{|y|^2}{|x+y|+|x|}-\frac{|y|^2}{2|x|} \lesssim \frac{|y|^3}{|x|^2}.$$

Therefore,

$$\left||x+y|-|x|-\frac{xy}{|x|}-\frac{|y|^2}{2|x|}+\frac{(xy)^2}{2|x|^3}\right| \lesssim \frac{|y|^3}{|x|^2}. \tag{2-5}$$

By (2-4) and (2-5), we then obtain (2-2). □

We can now establish the asymptotic expansion of eigenfunctions.

Lemma 2.5. *Assume that $V \in L^1 \cap L^{\frac{3}{2},1}$. Let $\phi \in \mathcal{E}$ be a zero-energy eigenfunction of H. Then*

$$\phi(x)-\sum_{k=1}^{3}\langle V\phi, y_k\rangle\frac{x_k}{|x|^3} \in |x|^{-2}(L^{3,\infty}\cap L^\infty).$$

Further assume that $V \in \langle x\rangle^{-1}L^1 \cap L^{\frac{3}{2},1}$. Then

$$\phi(x)-\sum_{k=1}^{3}\langle V\phi, y_k\rangle\frac{x_k}{|x|^3}-\sum_{k,\ell=1}^{3}\langle \phi V, y_k y_\ell\rangle\left(\frac{\delta_{k\ell}}{2|x|^3}-\frac{3x_k x_\ell}{2|x|^5}\right) \in |x|^{-3}(L^{3,\infty}\cap L^\infty).$$

In particular, $\phi \in \mathcal{E}$ is in L^1 if and only if $\langle V\phi, y_k\rangle = 0$ and $\langle V\phi, y_k y_\ell\rangle = 0$ for $1 \le k, \ell \le 3$.

Let $\mathcal{E}_1 := \mathcal{E} \cap L^1$. Then $\operatorname{codim}_{\mathcal{E}} \mathcal{E}_1 \le 12$.

Proof of Lemma 2.5. We start from the eigenfunction equation

$$\phi(x) = -\frac{1}{4\pi}\int_{\mathbb{R}^3}\frac{1}{|x-y|}V(y)\phi(y)\,dy.$$

Recall that $\langle \phi, V\rangle = 0$. Using (2-1), we obtain that

$$\left|\phi(x)-\sum_{k=1}^{3}\langle V\phi, y_k\rangle\frac{x_k}{|x|^3}\right| \lesssim \frac{1}{|x|^2}\int_{\mathbb{R}^3}\frac{|y|^2|V(y)||\phi(y)|\,dy}{|x-y|}.$$

Since $\phi \in \langle x\rangle^{-2}L^\infty$ and $V \in L^1 \cap L^{\frac{3}{2},1}$, the right-hand side is in $|x|^{-2}(L^{3,\infty}\cap L^\infty)$.

Using (2-2), we obtain instead that

$$\left|\phi(x) - \sum_{k=1}^{3} \langle \phi V, y_k\rangle \frac{x_k}{|x|^3} - \sum_{k,\ell=1}^{3} \langle \phi V, y_k y_\ell\rangle \left(\frac{\delta_{k\ell}}{2|x|^3} - \frac{3x_k x_\ell}{2|x|^5}\right)\right| \lesssim \frac{1}{|x|^3} \int_{\mathbb{R}^3} \frac{|y|^3 |V(y)|\,|\phi(y)|\,dy}{|x-y|}.$$

Since $\phi \in \langle x\rangle^{-2} L^\infty$ and $V \in \langle x\rangle^{-1} L^1 \cap L^{\frac{3}{2},1}$, the right-hand side is in $|x|^{-3}(L^{3,\infty} \cap L^\infty)$.

These estimates matter only in the region $\{x : |x| \geq 1\}$, since near zero, $\phi \in L^\infty \subset L^1(\{|x| \leq 1\})$. As $|x|^{-3} L^{3,\infty} \subset L^1(\{|x| \geq 1\})$ and

$$\frac{x_k}{|x|^3},\ \frac{\delta_{k\ell}}{2|x|^3} - \frac{3x_k x_\ell}{2|x|^5} \notin L^1$$

are linearly independent, it follows that $\phi \in \mathcal{E}$ is in L^1 if and only if all the coefficients $\langle V\phi, y_k\rangle$ and $\langle V\phi, y_k y_\ell\rangle$ are zero.

Then $\mathcal{E}_1$ is the kernel of a rank-12 map $\phi \mapsto \big(\langle \phi V, y_k\rangle, \langle \phi V, y_k y_\ell\rangle\big)$ from $\mathcal{E}$ to $\mathbb{C}^{12}$, so $\operatorname{codim}_{\mathcal{E}} \mathcal{E}_1 \leq 12$. □

2C. *Wiener spaces.*

Definition. For a Banach lattice X, let the space $\mathcal{V}_X$ consist of kernels $T(x, y, \sigma)$ such that, for each pair (x, y), we have that $T(x, y, \sigma)$ is a finite measure in σ on $\mathbb{R}$ and

$$M(T)(x, y) := \int_{\mathbb{R}} d|T(x, y, \sigma)|$$

is an X-bounded operator.

$\mathcal{V}_X$ is an algebra under

$$(T_1 * T_2)(x, z, \sigma) := \int T_1(x, y, \rho) T_2(y, z, \sigma - \rho)\,dy\,ds.$$

Elements of $\mathcal{V}_X$ have Fourier transforms

$$\widehat{T}(x, y, \lambda) := \int_{\mathbb{R}} e^{-i\sigma\lambda}\,dT(x, y, \sigma),$$

which are uniformly X-bounded operators, $\widehat{T}(\lambda) \in L^\infty_\lambda \mathcal{B}(X)$, and, for every $\lambda \in \mathbb{R}$, we have $\widehat{T}_1(\lambda)\widehat{T}_2(\lambda) = (T_1 * T_2)^\wedge(\lambda)$.

The space $\mathcal{V}_X$ contains elements of the form $\delta_0(\sigma) T(x, y)$, whose Fourier transform is constantly the operator $T(x, y) \in \mathcal{B}(X)$. In particular, rank-one operators $\delta_0(\sigma)\phi(x) \otimes \psi(y)$ are in $\mathcal{V}_X$ when $\psi \in X^*$ and $\phi \in X$. More generally, $f(\sigma) T(x, y) \in \mathcal{V}_X$ if $f \in L^1$ and $T \in \mathcal{B}(X)$.

Moreover, for two Banach lattices X and Y of functions on $\mathbb{R}^3$, we also define the space $\mathcal{V}_{X,Y}$ of kernels $T(x, y, \sigma)$ such that $M(T)(x, y)$ is a bounded operator from X to Y. The category of such operators forms an algebroid, in the sense that

$$\|T_1 * T_2\|_{\mathcal{V}_{X,Z}} \leq \|T_1\|_{\mathcal{V}_{Y,Z}} \|T_2\|_{\mathcal{V}_{X,Y}}.$$

For example, note that

$$\big(R_0((\lambda + i0)^2)\big)^\wedge \in \mathcal{V}_{L^{3/2,1}, L^\infty} \cap \mathcal{V}_{L^1, L^{3,\infty}} \quad \text{and} \quad \big(\partial_\lambda R_0((\lambda + i0)^2)\big)^\wedge \in \mathcal{V}_{L^1, L^\infty}.$$

Indeed, the Fourier transform in λ is

$$\big(R_0((\lambda+i0)^2)\big)^\wedge(\sigma)(x,y) = (4\pi\sigma)^{-1}\delta_{|x-y|}(\sigma),$$

so we have

$$M\big(\big(R_0((\lambda+i0)^2)\big)^\wedge\big) = \frac{1}{4\pi|x-y|}.$$

Clearly $1/(4\pi|x-y|)$ is in $\mathcal{B}(L^{\frac{3}{2},1}, L^\infty) \cap \mathcal{B}(L^1, L^{3,\infty})$.

Likewise,

$$\big(\partial_\lambda R_0((\lambda+i0)^2)\big)^\wedge(\sigma)(x,y) = (4\pi)^{-1} i\,\delta_{|x-y|}(\sigma),$$

so we have

$$M\big(\big(\partial_\lambda R_0((\lambda+i0)^2)\big)^\wedge\big) = (4\pi)^{-1} 1 \otimes 1,$$

which is in $\mathcal{B}(L^1, L^\infty)$.

A space that will repeatedly intervene in computations is

$$\mathcal{W} = \big\{L \mid L^\vee \in \mathcal{V}_{L^{3/2,2}} \cap \mathcal{V}_{L^{3,2}},\ (\partial_\lambda L)^\vee \in \mathcal{V}_{L^{3/2,2},L^{3,2}}\big\}.$$

This space has the algebra property that $L_1, L_2 \in \mathcal{W} \Longrightarrow L_1(\lambda)L_2(\lambda) \in \mathcal{W}$.

The following technical lemma will be useful:

Lemma 2.6 (Fourier transforms).

$$M\bigg(\bigg(\frac{e^{is|x-y|}}{4\pi|x-y|}\bigg)^\wedge\bigg) = \frac{1}{4\pi|x-y|},$$

$$M\bigg(\bigg(\partial_s \frac{e^{is|x-y|}}{4\pi|x-y|}\bigg)^\wedge\bigg) = \frac{1\otimes 1}{4\pi},$$

$$M\bigg(\bigg(\frac{R_0((s+i0)^2)-R_0(0)}{s}\bigg)^\wedge\bigg) = \frac{1\otimes 1}{4\pi},$$

$$M\bigg(\bigg(\partial_s \frac{R_0((s+i0)^2)-R_0(0)}{s}\bigg)^\wedge\bigg) = \frac{|x-y|}{8\pi},$$

$$M\bigg(\bigg(\frac{R_0((s+i0)^2)-R_0(0)-is\frac{1\otimes 1}{4\pi}}{s^2}\bigg)^\wedge\bigg) = \frac{|x-y|}{8\pi},$$

$$M\bigg(\bigg(\partial_s \frac{R_0((s+i0)^2)-R_0(0)-is\frac{1\otimes 1}{4\pi}}{s^2}\bigg)^\wedge\bigg) = \frac{|x-y|^2}{24\pi}.$$

Proof. Let $a>0$. Observe that the Fourier transform of $e^{i\lambda a}$ in λ is $\delta_a(t)$. Then

$$\frac{e^{i\lambda a}-1}{i\lambda} = \int_0^a e^{i\lambda b}\,db,$$

so $\big((e^{i\lambda a}-1)/(i\lambda)\big)^\wedge = \chi_{[0,a]}(\lambda)$. Also

$$\frac{e^{i\lambda a}-1-i\lambda a}{i\lambda^2} = \int_0^a \frac{e^{i\lambda b}-1}{\lambda}\,db,$$

so $\big((e^{i\lambda a}-1-i\lambda a)/(i\lambda^2)\big)^\wedge=(a-t)\chi_{[0,a]}(t)$.

Note that

$$R_0((s+i0)^2)=\frac{e^{is|x-y|}}{4\pi|x-y|}$$

has the Fourier transform $\delta_{|x-y|}(\sigma)/(4\pi|x-y|)$. Thus

$$R_0\big((s+i0)^2\big)^\wedge=\left(\frac{e^{is|x-y|}}{4\pi|x-y|}\right)^\wedge=\frac{\delta_{|x-y|}(\sigma)}{4\pi|x-y|}.$$

Integrating the absolute value in σ, we obtain $1/(4\pi|x-y|)$.

Likewise,

$$\left(\frac{R_0((s+i0)^2)-R_0(0)}{s}\right)^\wedge=\frac{i\chi_{[0,|x-y|]}(\sigma)}{4\pi|x-y|}.$$

Integrating the absolute value in σ, we get $1/(4\pi)=(1\otimes 1)/(4\pi)$.

The Fourier transform of the derivative is

$$\left(\partial_s\frac{R_0((s+i0)^2)-R_0(0)}{s}\right)^\wedge=\frac{i\sigma\chi_{[0,|x-y|]}(\sigma)}{4\pi|x-y|}.$$

Integrating in σ, we obtain $|x-y|/(8\pi)$.

Next,

$$\left(\frac{R_0((s+i0)^2)-R_0(0)-is1\otimes 1}{s^2}\right)^\wedge=\left(\frac{e^{is|x-y|}-1-is|x-y|}{4\pi s^2|x-y|}\right)^\wedge=\frac{(|x-y|-\sigma)\chi_{[0,|x-y|]}(\sigma)}{4\pi|x-y|}. \tag{2-6}$$

Integrating in σ, we obtain $|x-y|/(8\pi)$.

The Fourier transform of the derivative is

$$\left(\partial_s\frac{R_0((s+i0)^2)-R_0(0)-is1\otimes 1}{s^2}\right)^\wedge=\frac{\sigma(|x-y|-\sigma)\chi_{[0,|x-y|]}(\sigma)}{4\pi|x-y|}.$$

Integrating in σ, we obtain $|x-y|^2/(24\pi)$. □

2D. ***Regular points and regular Hamiltonians.*** Before examining the possible singularity at zero, we study what happens at regular points in the spectrum.

Recall the notation $V_1=|V|^{\frac12}$ and $V_2=|V|^{\frac12}\operatorname{sgn}V$. The following two properties play an important part in the study:

Lemma 2.7. *Let*

$$T(x,y,\rho):=\frac{V_2(x)V_1(y)}{4\pi|x-y|}\delta_{-|x-y|}(\rho),$$

so $\widehat{T}(\lambda)=V_2R_0((\lambda+i0)^2)V_1$. *Then*:

(C1) $\lim_{R\to\infty}\|\chi_{\rho\geq R}(\rho)T(\rho)\|_{\mathcal{V}_{L^{3/2,2}}\cap\mathcal{V}_{L^{3,2}}}=0$.

(C2) *For some* $N\geq 1$, *we have* $\lim_{\epsilon\to 0}\|T^N(\rho+\epsilon)-T^N(\rho)\|_{\mathcal{V}_{L^{3/2,2}}\cap\mathcal{V}_{L^{3,2}}}=0$.

Here the powers of T mean repeated convolution. We refer the reader to similar properties that appear in the proof of [Beceanu and Goldberg 2012, Theorem 5].

Proof of Lemma 2.7. Suppose V_1 and V_2 are bounded functions with compact support in $B(0, D)$. It follows that for $R > 2D$, we have $\chi\big(\frac{t}{R}\big)T(t) = 0$, so in particular

$$\|\chi_{t\geq R}T\|_{\mathcal{V}_{L^{3/2,2}}\cap\mathcal{V}_{L^{3,2}}} \to 0$$

as $R \to \infty$, and property (C1) is preserved by taking the limits of V_1 and V_2 in $L^{3,2}$.

Next, fix $p \in \big(1, \frac{4}{3}\big]$ and assume that V_1 and V_2 are bounded and of compact support.

Since V_1 and V_2 are bounded and of compact support, T also has the local and distal properties

$$\lim_{\epsilon\to 0}\left\|\chi_{<\epsilon}(|x-y|)\frac{V_2(x)V_1(y)}{|x-y|}\right\|_{\mathcal{B}(L^{3/2,2})\cap\mathcal{B}(L^{3,2})} = 0,$$
$$\lim_{R\to\infty}\left\|\chi_{>R}(|x-y|)\frac{V_2(x)V_1(y)}{|x-y|}\right\|_{\mathcal{B}(L^{3/2,2})\cap\mathcal{B}(L^{3,2})} = 0.$$

Combined with condition (C1), this implies that for any $\epsilon > 0$ there exists a cutoff function χ compactly supported in $(0, \infty)$ such that

$$\|\chi(\rho)T(\rho) - T(\rho)\|_{\mathcal{V}_{L^{3/2,2}}\cap\mathcal{V}_{L^{3,2}}} < \epsilon.$$

Thus, it suffices to show that condition (C2) holds for $\chi(\rho)T(\rho)$.

The Fourier transform of $\chi(\rho)T(\rho)$ has the form

$$\big(\chi(\rho)T(\rho)\big)^\wedge(\lambda) = V_2(x)\frac{e^{i\lambda|x-y|}}{4\pi|x-y|}\chi(|x-y|)V_1(y). \tag{2-7}$$

Such oscillating kernels have decay in the L^p operator norm for $p > 1$. By [Stein 1993, Lemma on p. 392], with p' being the dual exponent, that is, we have $\frac{1}{p} + \frac{1}{p'} = 1$,

$$\big\|(\chi(\rho)T(\rho))^\wedge(\lambda)f\big\|_{L^p} \lesssim \lambda^{-\frac{3}{p'}}\|f\|_{L^p}. \tag{2-8}$$

Taking into account the fact that $(\chi(\rho)T(\rho))^\wedge(\lambda)$ has a kernel bounded in absolute value by

$$\frac{|V(x)|^{\frac{1}{2}}|V(y)|^{\frac{1}{2}}}{4\pi|x-y|}$$

(where $|V|^{\frac{1}{2}} = V_1$ is bounded and has compact support by assumption), it follows that $(\chi(\rho)T(\rho))^\wedge(\lambda)$ is uniformly bounded in $\mathcal{B}(X, L^p)$, $\mathcal{B}(L^p, X)$, and $\mathcal{B}(L^p)$ for all λ, where X is $L^{\frac{3}{2},2}$ or $L^{3,2}$. Therefore, by also using (2-8) for the middle factors,

$$\big\|\big((\chi(\rho)T(\rho))^\wedge(\lambda)\big)^N f\big\|_X \lesssim \langle\lambda\rangle^{-\frac{3(N-2)}{p'}}\|f\|_X.$$

For $N > 2 + \frac{2p'}{3}$, this shows that $\partial_\rho(\chi(\rho)T(\rho))^N$ are uniformly bounded operators in $\mathcal{B}(X)$, where X is either $L^{\frac{3}{2},2}$ or $L^{3,2}$. Since $\big(\chi(\rho)T(\rho)\big)^N$ has compact support in ρ, this in turn implies (C2).

For general $V \in L^{\frac{3}{2},1}$, choose a sequence of bounded compactly supported approximations for which (C2) holds, as shown above. By a limiting process, we obtain that (C2) also holds for V. ☐

Lemma 2.8. *Let $\widehat{T}(\lambda) = V_2 R_0((\lambda + i0)^2)V_1$. Assume that $V \in L^{\frac{3}{2},1}$ and let $\lambda_0 \neq 0$. Consider a cutoff function χ. Then, for $\epsilon \ll 1$, we have*

$$\chi\Big(\frac{\lambda-\lambda_0}{\epsilon}\Big)(I + \widehat{T}(\lambda))^{-1} \in \mathcal{W}.$$

The same holds for $\lambda_0 = 0$ if V is a generic potential.

Infinity has the same property: for $R \gg 1$, we have

$$\Big(1 - \chi\Big(\frac{\lambda}{R}\Big)\Big)(I + \widehat{T}(\lambda))^{-1} \in \mathcal{W}.$$

Proof of Lemma 2.8. Note that $I + \widehat{T}(\lambda_0)$ is invertible in $\mathcal{B}(L^{\frac{3}{2},2})$ and in $\mathcal{B}(L^{3,2})$ for all $\lambda_0 \neq 0$, the only issue being at zero.

Indeed, assume that $I + \widehat{T}(\lambda_0)$ is not invertible in $\mathcal{B}(L^{\frac{3}{2},2})$; then, by Fredholm's alternative, there exists a nonzero $f \in L^{\frac{3}{2},2}$ such that

$$f = -V_2 R_0((\lambda_0 + i0)^2)V_1 f.$$

Let $V_1 = V_1^1 + V_1^2$ and $V_2 = V_2^1 + V_2^2$, where V_1^1 and V_2^1 have compact support and are bounded with $\|V_1^2\|_{L^{3,2}}, \|V_2^2\|_{L^{3,2}} \ll 1$. Then

$$f = -\big(I + V_2 R_0((\lambda_0 + i0)^2)V_1^2 + V_2^2 R_0((\lambda_0 + i0)^2)V_1^1\big)^{-1} V_2^1 R_0((\lambda_0 + i0)^2)V_1^1 f,$$

which implies that $f \in L^2$. Letting $g = R_0((\lambda_0 + i0)^2)V_1 f$, we obtain a nonzero $L^{6,\infty}$ solution g of the equation

$$g = -R_0((\lambda_0 + i0)^2)Vg.$$

However, this is impossible for $\lambda_0 \neq 0$ due to the results of Ionescu and Jerison [2003] and Goldberg and Schlag [2004b].

When $\lambda_0 = 0$, we have that g is a zero-energy eigenfunction or resonance for $H = -\Delta + V$, which cannot happen if V is a generic potential.

Let

$$S_\epsilon(\lambda) = \chi\Big(\frac{\lambda-\lambda_0}{\epsilon}\Big)(\widehat{T}(\lambda) - \widehat{T}(\lambda_0)).$$

A simple argument based on condition (C1) shows that $\lim_{\epsilon\to 0} \|S_\epsilon^\vee\|_{\mathcal{V}_{L^{3/2,2}} \cap \mathcal{V}_{L^{3,2}}} = 0$. Then

$$\begin{aligned}\chi\Big(\frac{\lambda-\lambda_0}{\epsilon}\Big)(I + \widehat{T}(\lambda))^{-1} &= \chi\Big(\frac{\lambda}{\epsilon}\Big)\Big(I + \widehat{T}(\lambda_0) + \chi\Big(\frac{\lambda-\lambda_0}{2\epsilon}\Big)(\widehat{T}(\lambda) - \widehat{T}(\lambda_0))\Big)^{-1} \\ &= \chi\Big(\frac{\lambda-\lambda_0}{\epsilon}\Big)(I + \widehat{T}(\lambda_0))^{-1} \sum_{k=0}^{\infty} (-1)^k \big(S_{2\epsilon}(\lambda)(I + \widehat{T}(\lambda_0))^{-1}\big)^k.\end{aligned}$$

The Fourier transform of the series above converges for sufficiently small ϵ, showing that

$$\Big(\chi\Big(\frac{\lambda-\lambda_0}{\epsilon}\Big)(I + \widehat{T}(\lambda))^{-1}\Big)^\vee \in \mathcal{V}_{L^{3/2,2}} \cap V_{L^{3,2}}.$$

Concerning the derivative,

$$\chi\Big(\frac{\lambda-\lambda_0}{\epsilon}\Big)\partial_\lambda(I + \widehat{T}(\lambda))^{-1} = -\chi\Big(\frac{\lambda-\lambda_0}{\epsilon}\Big)(I + \widehat{T}(\lambda))^{-1}\partial_\lambda \widehat{T}(\lambda)\chi\Big(\frac{\lambda-\lambda_0}{2\epsilon}\Big)(I + \widehat{T}(\lambda))^{-1}.$$

Here

$$\Big(\chi\Big(\frac{\lambda-\lambda_0}{2\epsilon}\Big)(I+\widehat{T}(\lambda))^{-1}\Big)^{\vee} \in \mathcal{V}_{L^{3/2,2}} \cap \mathcal{V}_{L^{3,2}} \quad \text{and} \quad (\partial_\lambda \widehat{T}(\lambda))^{\vee} \in \mathcal{V}_{L^{3/2,2},L^{3,2}}$$

since

$$M\big((\partial_\lambda T(\lambda))^{\vee}\big) = \frac{|V_2(x)| \otimes |V_1(y)|}{4\pi}.$$

Then

$$\Big(\chi\Big(\frac{\lambda-\lambda_0}{\epsilon}\Big)\partial_\lambda(I+\widehat{T}(\lambda))^{-1}\Big)^{\vee} \in \mathcal{V}_{L^{3/2,2},L^{3,2}}.$$

At infinity, for any real number L, one can express $\big(1-\chi\big(\frac{\lambda}{R}\big)\big)\widehat{T}(\lambda)$ as the Fourier transform of

$$S_R(\rho) = \big(T - R\check{\chi}(R\,\cdot) * T\big)(\rho) = \int_{\mathbb{R}} R\check{\chi}(R\sigma)\big[T(\rho) - T(\rho-\sigma)\big]\,d\sigma.$$

Thanks to condition (C2), the norm of the right-hand side integral vanishes as $L \to \infty$. This makes it possible to construct an inverse Fourier transform for

$$\Big(1-\chi\Big(\frac{\lambda}{R}\Big)\Big)(I+\widehat{T}(\lambda))^{-1} = \Big(1-\chi\Big(\frac{\lambda}{R}\Big)\Big)\sum_{k=0}^{\infty}(-1)^k\Big(\Big(1-\chi\Big(\frac{2\lambda}{R}\Big)\Big)\widehat{T}(\lambda)\Big)^k$$

via this power series expansion, which converges for sufficiently large R.

If only T^N satisfies (C2) then one constructs an inverse Fourier transform for

$$\Big(1-\chi\Big(\frac{\lambda}{R}\Big)\Big)(I-(-\widehat{T})^N(\lambda))^{-1}$$

in this manner and observes that

$$\Big(1-\chi\Big(\frac{\lambda}{R}\Big)\Big)(I+\widehat{T}(\lambda))^{-1} = \Big(1-\chi\Big(\frac{\lambda}{R}\Big)\Big)\big(I-(-\widehat{T}(\lambda))^N\big)^{-1}\sum_{k=0}^{N-1}(-1)^k\widehat{T}^k(\lambda).$$

Finally, concerning the derivative in a neighborhood of infinity, we note that

$$\Big(1-\chi\Big(\frac{\lambda}{R}\Big)\Big)\partial_\lambda(I+\widehat{T}(\lambda))^{-1} = -\Big(1-\chi\Big(\frac{\lambda}{R}\Big)\Big)(I+\widehat{T}(\lambda))^{-1}\partial_\lambda\widehat{T}(\lambda)\Big(1-\chi\Big(\frac{2\lambda}{R}\Big)\Big)(I+\widehat{T}(\lambda))^{-1}.$$

Here

$$\Big(\Big(1-\chi\Big(\frac{2\lambda}{R}\Big)\Big)(I+\widehat{T}(\lambda))^{-1}\Big)^{\vee} \in \mathcal{V}_{L^{3/2,2}} \cap \mathcal{V}_{L^{3,2}} \quad \text{and} \quad (\partial_\lambda \widehat{T}(\lambda))^{\vee} \in \mathcal{V}_{L^{3/2,2},L^{3,2}}.$$

Therefore,

$$\Big(\Big(1-\chi\Big(\frac{\lambda}{R}\Big)\Big)\partial_\lambda(I+\widehat{T}(\lambda))^{-1}\Big)^{\vee} \in \mathcal{V}_{L^{3/2,2},L^{3,2}}.$$

□

In the case when H is generic, we can cover the whole spectrum $[0,\infty)$ by open neighborhoods of regular points, plus an open neighborhood of infinity, and choose a subordinate partition of unity. We retrieve a form of [Beceanu and Goldberg 2012, Theorem 2]:

Theorem 2.9. *Let $V \in L^{\frac{3}{2},1}$ be a real-valued potential for which the Schrödinger operator $H = -\Delta + V$ has no resonances or eigenvalues at zero energy. Then*

$$\|e^{-itH}P_c f\|_\infty \lesssim |t|^{-\frac{3}{2}}\|f\|_1. \tag{2-9}$$

In the context of the wave equation, again if the Hamiltonian H is generic, we retrieve the results of [Beceanu and Goldberg 2014].

Proof of Theorem 2.9. Consider a sufficiently large R such that

$$\Big(1-\chi\Big(\frac{\lambda}{R}\Big)\Big)(I+\widehat{T}(\lambda))^{-1}\in\mathcal{W}$$

by Lemma 2.8. Also by Lemma 2.8, for every $\lambda_0\in[-4R,4R]$ (including zero, since V is a generic potential), there exists $\epsilon(\lambda_0)>0$ such that

$$\chi\Big(\frac{\lambda-\lambda_0}{\epsilon(\lambda_0)}\Big)(I+\widehat{T}(\lambda))^{-1}\in\mathcal{W}.$$

Since $[-4R,4R]$ is a compact set, there exists a finite covering

$$[-4R,4R]\subset\bigcup_{k=1}^{N}\big(\lambda_k-\epsilon(\lambda_k),\lambda_k+\epsilon(\lambda_k)\big).$$

Then we construct a finite partition of unity on $\mathbb{R}$ by smooth functions $1=\sum_{k=1}^{N}\chi_k(\lambda)+\chi_\infty(\lambda)$, where $\operatorname{supp}\chi_\infty\subset\mathbb{R}\setminus(-2R,2R)$ and $\operatorname{supp}\chi_k\subset\big[\lambda_k-\epsilon(\lambda_k),\lambda_k+\epsilon(\lambda_k)\big]$. By our construction, for each $1\le k\le N$ and for $k=\infty$, we have $\chi_k(\lambda)(I+\widehat{T}(\lambda))^{-1}\in\mathcal{W}$, so summing up we obtain that $(I+\widehat{T}(\lambda))^{-1}\in\mathcal{W}$.

By spectral calculus, we express the perturbed evolution as

$$\begin{aligned}
e^{itH}P_cf&=\frac{1}{2\pi i}\int_0^\infty e^{it\lambda}\big(R_V(\lambda+i0)-R_V(\lambda-i0)\big)f\,d\lambda\\
&=\frac{1}{\pi i}\int_{-\infty}^{\infty}e^{it\lambda^2}R_V((\lambda+i0)^2)f\lambda\,d\lambda\\
&=\frac{1}{\pi i}\int_{-\infty}^{\infty}e^{it\lambda^2}\big(R_0((\lambda+i0)^2)-R_0((\lambda+i0)^2)V_1(I+\widehat{T}(\lambda))^{-1}V_2R_0((\lambda+i0)^2)\big)f\lambda\,d\lambda\\
&=\frac{1}{2\pi t}\int_{-\infty}^{\infty}e^{it\lambda^2}\partial_\lambda\big(R_0((\lambda+i0)^2)-R_0((\lambda+i0)^2)V_1(I+\widehat{T}(\lambda))^{-1}V_2R_0((\lambda+i0)^2)\big)f\,d\lambda\\
&=\frac{C}{t^{\frac32}}\int_{-\infty}^{\infty}e^{i\frac{\rho^2}{4t}}\big(\partial_\lambda\big(R_0((\lambda+i0)^2)-R_0((\lambda+i0)^2)V_1(I+\widehat{T}(\lambda))^{-1}V_2R_0((\lambda+i0)^2)\big)\big)^\vee(\rho)f\,d\rho.
\end{aligned}\tag{2-10}$$

Since $(I+\widehat{T}(\lambda))^{-1}\in\mathcal{W}$, it follows that $\big(\partial_\lambda(I+\widehat{T}(\lambda))^{-1}\big)^\vee\in\mathcal{V}_{L^{3/2,2},L^{3,2}}$. Taking into account that $R_0((\lambda+i0)^2)V_1\in\mathcal{V}_{L^1,L^{3/2,2}}$ and $V_2R_0((\lambda+i0)^2)\in\mathcal{V}_{L^{3,2},L^\infty}$, we obtain that

$$R_0((\lambda+i0)^2)V_1(I+\widehat{T}(\lambda))^{-1}V_2R_0((\lambda+i0)^2)\in\mathcal{V}_{L^1,L^\infty}.$$

By definition, this ensures a bound of $|t|^{-\frac32}$ for this expression's contribution to (2-10). The other terms are handled similarly. □

We next consider the effect of singularities at zero.

2E. *Exceptional Hamiltonians of the first kind.*

Let

$$Q=-\frac{1}{2\pi i}\int_{|z+1|=\delta}\big(V_2R_0(0)V_1-zI\big)^{-1}\,dz$$

and $\overline{Q} = 1 - Q$. Assuming that $H = -\Delta + V$ has only a resonance ϕ at zero, then (recalling that $-\langle \phi, V\phi \rangle = 1$), by the analytic Fredholm theorem,

$$Q = -V_2\phi \otimes V_1\phi.$$

The resonance $\phi \in \mathcal{M}$ satisfies the equation $\phi = -R_0(0)V\phi$. Since $\phi \in L^{3,\infty} \cap L^\infty$, we have that Q is bounded on $L^{\frac{3}{2},2}$ and on $L^{3,2}$, so the constant family of operators Q is in $\mathcal{W}$. Moreover, Q is in $\mathcal{B}(L^{\frac{3}{2},2}, L^{3,2})$ and in $\mathcal{B}(L^{3,2}, L^{\frac{3}{2},2})$.

Note that, since

$$e^{i\lambda|x-y|} - 1 \lesssim \min(1, \lambda|x-y|) \quad \Longrightarrow \quad e^{i\lambda|x-y|} - 1 \lesssim \lambda^\delta |x-y|^\delta,$$

one has

$$V_2(x)\left(\frac{e^{i\lambda|x-y|}}{|x-y|} - \frac{1}{|x-y|}\right)V_1(y) \lesssim |V_2(x)|\lambda|V_1(y)|. \tag{2-11}$$

Thus, when $V \in \langle x\rangle^{-1} L^{\frac{3}{2},1}$,

$$I + \widehat{T}(\lambda) = I + V_2 R_0((\lambda + i0)^2)V_1$$

is Lipschitz continuous in $\mathcal{B}(L^2)$. This implies that, more generally, when $V \in L^{\frac{3}{2},1}$, we have that $\widehat{T}(\lambda)$ is continuous in $\mathcal{B}(L^2)$ (the proof is by approximation).

In a similar manner, by approximating $V \in L^{\frac{3}{2},1}$ with $\langle x\rangle^{-2} L^{\frac{3}{2},1}$ potentials, we obtain that $\widehat{T}(\lambda)$ is continuous in $\mathcal{B}(L^{\frac{3}{2},2}) \cap \mathcal{B}(L^{3,2})$.

Let

$$K = \big(I + V_2 R_0(0) V_1 + Q\big)^{-1} \overline{Q}.$$

Then K is the inverse of $\overline{Q}(I + \widehat{T}(0))\overline{Q} = \overline{Q}\big(I + V_2 R_0(0)V_1\big)\overline{Q}$ in $\mathcal{B}(\overline{Q}L^{\frac{3}{2},2} \cap \overline{Q}L^{3,2})$, in the sense that

$$K\overline{Q}\big(I + V_2 R_0(0)V_1\big)\overline{Q} = \overline{Q}\big(I + V_2 R_0(0)V_1\big)\overline{Q}K = \overline{Q}. \tag{2-12}$$

By continuity, $\overline{Q}\big(I + V_2 R_0((\lambda + i0)^2)V_1\big)\overline{Q}$ is also invertible for $|\lambda| \ll 1$.

The following lemma, also known as the Feshbach lemma, is extremely useful in studying the singularity at zero.

Lemma 2.10 (see [Yajima 2005, Lemma 4.7]). *Let $X = X_0 + X_1$ be a direct sum decomposition of a vector space X. Suppose that a linear operator $L \in \mathcal{B}(X)$ is written in the form*

$$L = \begin{pmatrix} L_{00} & L_{01} \\ L_{10} & L_{11} \end{pmatrix}$$

with respect to this decomposition and that L_{00}^{-1} exists. Set $C = L_{11} - L_{10}L_{00}^{-1}L_{01}$. Then, L^{-1} exists if and only if C^{-1} exists. In this case,

$$L^{-1} = \begin{pmatrix} L_{00}^{-1} + L_{00}^{-1}L_{01}C^{-1}L_{10}L_{00}^{-1} & -L_{00}^{-1}L_{01}C^{-1} \\ -C^{-1}L_{10}L_{00}^{-1} & C^{-1} \end{pmatrix}. \tag{2-13}$$

By definition, an exceptional point $\lambda \in \mathbb{C}$ is one where $I + V_2 R_0(\lambda)V_1$ is not L^2-invertible.

Lemma 2.11. *Assume that $V \in \langle x\rangle^{-2} L^{\frac{3}{2},1} \subset \langle x\rangle^{-1} L^1 \cap L^{\frac{3}{2},1}$ and that $H = -\Delta + V$ is exceptional of the first type, with a resonance ϕ at zero. Let χ be a fixed cutoff function. Then, for some $\epsilon > 0$,*

$$\chi\Big(\frac{\lambda}{\epsilon}\Big)(I + \widehat{T}(\lambda))^{-1} = L(\lambda) - \lambda^{-1}\chi\Big(\frac{\lambda}{\epsilon}\Big)\frac{4\pi i}{|\langle V, \phi\rangle|^2} V_2\phi \otimes V_1\phi,$$

where $L \in \mathcal{W}$.

Moreover, zero is an isolated exceptional point, so $H = -\Delta + V$ has finitely many negative eigenvalues.

The computations in the proof of this lemma parallel those in [Yajima 2005, Section 4.3]. The main difference is using $\widehat{L}^1$-related spaces instead of Hölder spaces.

Proof of Lemma 2.11. We apply Lemma 2.10 to

$$I + \widehat{T}(\lambda) := \begin{pmatrix} \overline{Q}(I + \widehat{T}(\lambda))\overline{Q} & \overline{Q}\widehat{T}(\lambda)Q \\ Q\widehat{T}(\lambda)\overline{Q} & Q(I + \widehat{T}(\lambda))Q \end{pmatrix} = \begin{pmatrix} T_{00}(\lambda) & T_{01}(\lambda) \\ T_{10}(\lambda) & T_{11}(\lambda) \end{pmatrix}.$$

Note that $T_{00}(\lambda) := \overline{Q}\big(I + V_2 R_0((\lambda + i0)^2) V_1\big)\overline{Q}$ is invertible in $\mathcal{B}(\overline{Q}L^{\frac{3}{2},2}) \cap \mathcal{B}(\overline{Q}L^{3,2})$ for $|\lambda| \ll 1$ because

$$T_{00}(0) = \overline{Q}(I + \widehat{T}(0))\overline{Q} = \overline{Q}\big(I + V_2 R_0(0) V_1\big)\overline{Q}$$

is invertible on $\overline{Q}L^{\frac{3}{2},2}$ and on $\overline{Q}L^{3,2}$ with inverse K (see (2-12)), and $T_{00}(\lambda)$ is continuous in the norm of $\mathcal{B}(\overline{Q}L^{\frac{3}{2},2}) \cap \mathcal{B}(\overline{Q}L^{3,2})$ (see (2-11) above).

Furthermore, start from

$$(R_0((\lambda + i0)^2))^\wedge \in \mathcal{V}_{L^{3/2,1}, L^\infty} \cap \mathcal{V}_{L^1, L^{3,\infty}} \quad \text{and} \quad (\partial_\lambda R_0((\lambda + i0)^2))^\wedge \in \mathcal{V}_{L^1, L^\infty}.$$

We know that

$$|V|^{\frac{1}{2}} \in \mathcal{B}(L^{\frac{3}{2},2}, L^1) \cap \mathcal{B}(L^\infty, L^{3,2}) \cap \mathcal{B}(L^{3,\infty}, L^{\frac{3}{2},2}) \cap \mathcal{B}(L^{3,2}, L^{\frac{3}{2},1}).$$

Thus $V_2 R_0((\lambda + i0)^2) V_1 \in \mathcal{W}$ and $\overline{Q}$ preserves that. Then $T_{00}(\lambda) \in \mathcal{W}$ as well.

Next, since $T_{00}(0)$ is invertible, for small ϵ we have $\chi\big(\frac{\lambda}{\epsilon}\big)T_{00}^{-1}(\lambda) \in \mathcal{W}$. The proof is as follows: Let

$$S_\epsilon(\lambda) := \chi\Big(\frac{\lambda}{\epsilon}\Big)\overline{Q}(\widehat{T}(\lambda) - \widehat{T}(0))\overline{Q}.$$

A simple argument based on condition (C1) shows that $\lim_{\epsilon \to 0} \|S_\epsilon^\vee\|_{\mathcal{V}_{L^{3/2,2}} \cap \mathcal{V}_{L^{3,2}}} = 0$. Then

$$\begin{aligned} \chi\Big(\frac{\lambda}{\epsilon}\Big)T_{00}^{-1}(\lambda) &= \chi\Big(\frac{\lambda}{\epsilon}\Big)\Big(T_{00}(0) + \chi\Big(\frac{\lambda}{2\epsilon}\Big)\overline{Q}(\widehat{T}(\lambda) - \widehat{T}(0))\overline{Q}\Big)^{-1} \\ &= \chi\Big(\frac{\lambda}{\epsilon}\Big)T_{00}^{-1}(0)\sum_{k=0}^{\infty}(-1)^k (S_{2\epsilon}(\lambda)T_{00}^{-1}(0))^k. \end{aligned}$$

The series above converges for sufficiently small ϵ, showing that $\chi\big(\frac{\lambda}{\epsilon}\big)T_{00}^{-1}(\lambda) \in \mathcal{V}_{L^{3/2,2}} \cap \mathcal{V}_{L^{3,2}}$.

Concerning the derivative,

$$\chi\Big(\frac{\lambda}{\epsilon}\Big)\partial_\lambda T_{00}^{-1}(\lambda) = -\chi\Big(\frac{\lambda}{\epsilon}\Big)T_{00}^{-1}(\lambda)\partial_\lambda T_{00}(\lambda)\chi\Big(\frac{\lambda}{2\epsilon}\Big)T_{00}^{-1}(\lambda).$$

In this expression, $\big(\chi\big(\frac{\lambda}{2\epsilon}\big)T_{00}^{-1}(\lambda)\big)^\vee \in \mathcal{V}_{L^{3/2,2}} \cap \mathcal{V}_{L^{3,2}}$ and $(\partial_\lambda T_{00}(\lambda))^\vee \in \mathcal{V}_{L^{3/2,2},L^{3,2}}$. Thus

$$\Big(\chi\Big(\frac{\lambda}{\epsilon}\Big)\partial_\lambda T_{00}^{-1}(\lambda)\Big)^\vee \in \mathcal{V}_{L^{3/2,2},L^{3,2}}.$$

This computation shows that $\chi\big(\frac{\lambda}{\epsilon}\big)T_{00}^{-1}(\lambda) \in \mathcal{W}$.

Let

$$\begin{aligned} J(\lambda) &:= \frac{\widehat{T}(\lambda) - \big(V_2 R_0(0) V_1 + i\lambda(4\pi)^{-1} V_2 \otimes V_1\big)}{\lambda^2} \\ &= \frac{V_2 R_0((\lambda+i0)^2)V_1 - V_2 R_0(0)V_1 - i\lambda(4\pi)^{-1} V_2 \otimes V_1}{\lambda^2}. \end{aligned}$$

Then (recall that $Q = -V_2\phi \otimes V_1\phi$),

$$\begin{aligned} T_{11}(\lambda) &= Q(I + \widehat{T}(\lambda))Q = Q\big(I + V_2 R_0((\lambda+i0)^2)V_1\big)Q \\ &= Q\big(V_2 R_0((\lambda+i0)^2)V_1 - V_2 R_0(0) V_1\big)Q \\ &= V_2\phi \otimes V\phi(R_0((\lambda+i0)^2) - R_0(0))V\phi \otimes V_1\phi \\ &= \Big(\lambda\frac{|\langle V,\phi\rangle|^2}{4i\pi} - \lambda^2\langle V_1\phi, J(\lambda)V_2\phi\rangle\Big)Q \\ &= \big(\lambda a^{-1} - \lambda^2\langle V_1\phi, J(\lambda)V_2\phi\rangle\big)Q \\ &=: \lambda c_0(\lambda)Q. \end{aligned} \tag{2-14}$$

Note that $c_0(0) = a^{-1} \neq 0$. Recall that $a = 4i\pi/|\langle V,\phi\rangle|^2$.

By the third line of (2-14), $c_0(\lambda) \in \widehat{L}^1$ if

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} V(x)\phi(x)V(y)\phi(y)\Big\|\frac{e^{i\lambda|x-y|}-1}{\lambda|x-y|}\Big\|_{\widehat{L}^1_\lambda}\,dx\,dy < \infty.$$

For every x and y, by Lemma 2.6,

$$\Big\|\frac{e^{i\lambda|x-y|}-1}{\lambda|x-y|}\Big\|_{\widehat{L}^1_\lambda} = \Big\|\frac{\chi_{[0,|x-y|]}(t)}{|x-y|}\Big\|_{L^1_t} = 1,$$

so it is enough to assume that $V\phi \in L^1$, i.e., that $V \in L^{\frac{3}{2},1}$, to prove that $c_0(\lambda) \in \widehat{L}^1$.

In order for $\partial_\lambda c_0(\lambda)$ to be in $\widehat{L}^1$, it suffices that

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} V(x)\phi(x)V(y)\phi(y)\Big\|\partial_\lambda\frac{e^{i\lambda|x-y|}-1}{\lambda|x-y|}\Big\|_{\widehat{L}^1_\lambda}\,dx\,dy < \infty.$$

For every x and y, by Lemma 2.6,

$$\Big\|\partial_\lambda\frac{e^{i\lambda|x-y|}-1}{\lambda|x-y|}\Big\|_{\widehat{L}^1_\lambda} = \Big\|\frac{t\chi_{[0,|x-y|]}(t)}{|x-y|}\Big\|_{L^1_t} = \frac{|x-y|}{2},$$

so $\partial_\lambda c_0(\lambda) \in \widehat{L}^1$ when $V\phi \in \langle x\rangle^{-1}L^1$, i.e., when $V \in L^1$.

Regarding $J(\lambda)$, if $V \in L^1$ then

$$\langle J(\lambda)V_2\phi, V_1\phi\rangle = \left\langle \frac{R_0((\lambda+i0)^2) - R_0(0) - i\lambda(4\pi)^{-1} 1\otimes 1}{\lambda^2} V\phi, V\phi\right\rangle \in \widehat{L}^1_\lambda. \tag{2-15}$$

Moreover, when $V \in \langle x\rangle^{-1}L^1$, we know $\langle \partial_\lambda J(\lambda)V_2\phi, V_1\phi\rangle \in \widehat{L}^1_\lambda$.

Furthermore, considering the fact that $\phi + R_0(0)V\phi = 0$, let us define

$$\begin{aligned}\lambda\tilde{\psi}(\lambda) &:= (I+\widehat{T}(\lambda))V_2\phi = \big(V_2R_0((\lambda+i0)^2)V - V_2R_0(0)V\big)\phi \\ &= \lambda\left(i\frac{V_2\otimes V_1}{4\pi} + \lambda J(\lambda)\right)V_2\phi\end{aligned}$$

and

$$\begin{aligned}\lambda\tilde{\psi}^*(\lambda) &:= (I+\widehat{T}(\lambda)^*)V_1\phi = \big(V_1R_0^*((\lambda+i0)^2)V - V_1R_0(0)V\big)\phi \\ &= \lambda\left(-i\frac{V_1\otimes V_2}{4\pi} + \lambda J^*(\lambda)\right)V_1\phi.\end{aligned}$$

Note that

$$M(J(\lambda)^\vee) = |V_2(x)|\frac{|x-y|}{8\pi}|V_1(y)|$$

is a bounded operator from $L^{\frac{3}{2},2}$ to $L^{3,2}$, assuming that $V \in \langle x\rangle^{-2}L^{\frac{3}{2},1}$. Thus $J(\lambda)^\vee \in \mathcal{V}_{L^{3/2,2},L^{3,2}}$ and the same goes for $\lambda\partial_\lambda J(\lambda)$.

Moreover,

$$M\big((\lambda J(\lambda))^\vee\big) = \frac{|V_2|\otimes|V_1|}{2\pi}.$$

Thus $(\lambda J(\lambda))^\vee \in \mathcal{V}_{L^2}$ for $V \in L^1$ and $(\lambda J(\lambda))^\vee \in \mathcal{V}_{L^{3/2,2}} \cap \mathcal{V}_{L^{3,2}}$ when $V \in \langle x\rangle^{-2}L^{\frac{3}{2},1}$. Further note that $(\partial_\lambda(\lambda J(\lambda)))^\vee = (J(\lambda) + \lambda\partial_\lambda J(\lambda))^\vee \in \mathcal{V}_{L^{3/2,2},L^{3,2}}$. It follows that $\lambda J(\lambda) \in \mathcal{W}$.

Then (recalling that $Q = -V_2\phi\otimes V_1\phi$),

$$\begin{aligned}T_{01}(\lambda) &:= \overline{Q}\widehat{T}(\lambda)Q = \overline{Q}(I+\widehat{T}(\lambda))Q = (I+\widehat{T}(\lambda))Q - Q(I+\widehat{T}(\lambda))Q \\ &= -\lambda\tilde{\psi}(\lambda)\otimes V_1\phi - \lambda c_0(\lambda)Q \\ &= -\lambda(\tilde{\psi}(\lambda) + c_0(\lambda)V_2\phi)\otimes V_1\phi.\end{aligned}$$

Likewise,

$$T_{10}(\lambda) = -\lambda V_2\phi\otimes\big(\tilde{\psi}^*(\lambda) + \overline{c_0(\lambda)}V_1\phi\big).$$

By our above computations, it follows that $T_{01}(\lambda) = \lambda E_1(\lambda)$ and $T_{10}(\lambda) = \lambda E_2(\lambda)$ with $E_1, E_2 \in \mathcal{W}$.

Then $-T_{10}(\lambda)T_{00}^{-1}(\lambda)T_{01}(\lambda) = \lambda^2 c_1(\lambda)Q$, where

$$\begin{aligned}c_1(\lambda) &:= -\big\langle \tilde{\psi}^*(\lambda) + \overline{c_0(\lambda)}V_1\phi, T_{00}^{-1}(\lambda)\big(\tilde{\psi}(\lambda) + c_0(\lambda)V_2\phi\big)\big\rangle \\ &= -\left\langle\left(-i\frac{V_1\otimes V_2}{4\pi} + \lambda J^*(\lambda)\right)V_1\phi + \overline{c_0(\lambda)}V_1\phi, T_{00}^{-1}(\lambda)\left(\left(i\frac{V_2\otimes V_1}{4\pi} + \lambda J(\lambda)\right)V_2\phi + c_0(\lambda)V_2\phi\right)\right\rangle.\end{aligned} \tag{2-16}$$

For example, one of the terms in (2-16) has the form

$$\big\langle \lambda J^*(\lambda)V_1\phi, T_{00}^{-1}(\lambda)\lambda J(\lambda)V_2\phi\big\rangle. \tag{2-17}$$

Since $\lambda J(\lambda) \in \mathcal{W}$ and $\chi\big(\frac{\lambda}{\epsilon}\big) T_{00}^{-1}(\lambda) \in \mathcal{W}$ and since $V_1\phi,\ V_2\phi \in L^{\frac{3}{2},2} \cap L^{3,2}$, it immediately follows that $\chi\big(\frac{\lambda}{\epsilon}\big)$(2-17) is in $\widehat{L}^1$ and its derivative is also in $\widehat{L}^1$.

We then recognize from formula (2-16) that, for a cutoff function χ,

$$\chi\Big(\frac{\lambda}{\epsilon}\Big) c_1(\lambda) \in \widehat{L}^1 \quad \text{and} \quad \chi\Big(\frac{\lambda}{\epsilon}\Big) \partial_\lambda c_1(\lambda) \in \widehat{L}^1$$

when $V \in \langle x \rangle^{-2} L^{\frac{3}{2},1}$.

Let

$$C(\lambda) := T_{11}(\lambda) - T_{10}(\lambda) T_{00}^{-1}(\lambda) T_{01}(\lambda).$$

Then

$$C(\lambda) = \big(\lambda a^{-1} - \lambda^2 \langle V_1\phi, J(\lambda) V_2\phi \rangle + \lambda^2 c_1(\lambda)\big) Q =: \lambda a^{-1} Q + \lambda^2 c_2(\lambda) Q.$$

Thus $C(\lambda)/\lambda$ is invertible for $|\lambda| \ll 1$, and when $V \in \langle x \rangle^{-2} L^{\frac{3}{2},1}$ one has that

$$\begin{aligned} C^{-1}(\lambda) &= \frac{1}{\lambda a^{-1} + \lambda^2 c_2(\lambda)} Q \\ &= \left(\frac{1}{\lambda a^{-1}} + \frac{1}{\lambda a^{-1} + \lambda^2 c_2(\lambda)} - \frac{1}{\lambda a^{-1}} \right) Q \\ &= \left(\frac{a}{\lambda} - \frac{c_2(\lambda)}{\big(a^{-1} + \lambda c_2(\lambda)\big) a^{-1}} \right) Q \\ &=: a\lambda^{-1} Q + E(\lambda). \end{aligned}$$

By our computations, such as (2-15), $\chi\big(\frac{\lambda}{\epsilon}\big) c_2(\lambda) \in \widehat{L}^1$ and $\chi\big(\frac{\lambda}{\epsilon}\big) \partial_\lambda c_2(\lambda) \in \widehat{L}^1$. Therefore for sufficiently small ϵ, as $Q \in \mathcal{B}(L^{\frac{3}{2},2}) \cap B(L^{3,2}) \cap \mathcal{B}(L^{\frac{3}{2},2}, L^{3,2})$, it follows that $\chi\big(\frac{\lambda}{\epsilon}\big) E(\lambda) \in \mathcal{W}$.

The inverse of $I + \widehat{T}(\lambda)$ is then given for small λ by formula (2-13):

$$(I + \widehat{T})^{-1} = \begin{pmatrix} T_{00}^{-1} + T_{00}^{-1} T_{01} C^{-1} T_{10} T_{00}^{-1} & -T_{00}^{-1} T_{01} C^{-1} \\ -C^{-1} T_{10} T_{00}^{-1} & C^{-1} \end{pmatrix}.$$

Three of the matrix elements belong to $\mathcal{W}$ when localized by $\chi\big(\frac{\lambda}{\epsilon}\big)$. Indeed, recall that $\chi\big(\frac{\lambda}{\epsilon}\big) T_{00}^{-1}(\lambda) \in \mathcal{W}$, $T_{10}(\lambda) = \lambda E_1(\lambda)$ and $T_{01}(\lambda) = \lambda E_2(\lambda)$, while $C^{-1} = \lambda^{-1} E_3(\lambda)$, with $E_1, E_2, \chi\big(\frac{\lambda}{\epsilon}\big) E_3 \in \mathcal{W}$.

The fourth matrix element is C^{-1} in the lower-right corner, which is the sum of the regular term $\chi\big(\frac{\lambda}{\epsilon}\big) E(\lambda) \in \mathcal{W}$ and the singular term

$$a\lambda^{-1} \chi\Big(\frac{\lambda}{\epsilon}\Big) Q = -a\lambda^{-1} \chi\Big(\frac{\lambda}{\epsilon}\Big) V_2\phi \otimes V_1\phi.$$

As an aside, note that $\lambda^{-1}\big(1 - \chi\big(\frac{\lambda}{\epsilon}\big)\big) \in \widehat{L}^1$ and the same holds for its derivative. Thus we can also write the singular term as $a\lambda^{-1} Q$.

Further note that $(I + \widehat{T})^{-1}$ is well-defined on a whole cut neighborhood of zero by formula (2-13) above. Thus zero is an isolated exceptional point, so there are finitely many negative eigenvalues. $\square$

The next lemma shows what happens in the case when the potential has the critical rate of decay.

Lemma 2.12. *Assume that $V \in L^{\frac{3}{2},1}$ and that $H = -\Delta + V$ is exceptional of the first kind. Let χ be a standard cutoff function. Then*

$$\chi\Big(\frac{\lambda}{\epsilon}\Big)(I + \widehat{T}(\lambda))^{-1} = L(\lambda) + \lambda^{-1} S(\lambda),$$

with $L(\lambda) \in \mathcal{W}$ and $S(\lambda)^\vee \in \mathcal{V}_{L^{3,2},L^{3/2,2}}$ for sufficiently small $\epsilon > 0$.

Furthermore, 0 *is an isolated exceptional point*, *so H has finitely many negative eigenvalues.*

Proof of Lemma 2.12. We again apply Lemma 2.10 to

$$I + \widehat{T}(\lambda) := \begin{pmatrix} \overline{Q}(I + \widehat{T}(\lambda))\overline{Q} & \overline{Q}\widehat{T}(\lambda)Q \\ Q\widehat{T}(\lambda)\overline{Q} & Q(I + \widehat{T}(\lambda))Q \end{pmatrix} \equiv \begin{pmatrix} T_{00}(\lambda) & T_{01}(\lambda) \\ T_{10}(\lambda) & T_{11}(\lambda) \end{pmatrix}.$$

The proof of the fact that $\chi\big(\frac{\lambda}{\epsilon}\big)T_{00}^{-1}(\lambda) \in \mathcal{W}$ is the same as in Lemma 2.11.

Then note that

$$\begin{aligned} T_{11}(\lambda) &= Q(I + \widehat{T}(\lambda))Q = Q\big(I + V_2 R_0((\lambda + i0)^2)V_1\big)Q \\ &= Q\big(V_2 R_0((\lambda + i0)^2)V_1 - V_2 R_0(0)V_1\big)Q \\ &= V_2\phi \otimes V\phi\big(R_0((\lambda + i0)^2) - R_0(0)\big)V\phi \otimes V_1\phi \\ &=: \lambda c_0(\lambda) Q. \end{aligned}$$

Observe that $c_0(0) = a^{-1} \neq 0$. Recall that $a = 4i\pi/|\langle V, \phi\rangle|^2$.

Note that $c_0(\lambda) \in \widehat{L}^1$ if

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} V(x)\phi(x)V(y)\phi(y)\bigg\|\frac{e^{i\lambda|x-y|} - 1}{\lambda|x-y|}\bigg\|_{\widehat{L}^1_\lambda} dx\,dy < \infty.$$

For every x and y, by Lemma 2.6,

$$\bigg\|\frac{e^{i\lambda|x-y|} - 1}{\lambda|x-y|}\bigg\|_{\widehat{L}^1_\lambda} = \bigg\|\frac{\chi_{[0,|x-y|]}(t)}{|x-y|}\bigg\|_{L^1_t} = 1,$$

so it is enough to assume that $V\phi \in L^1$, i.e., that $V \in L^{\frac{3}{2},1}$, to prove that $c_0(\lambda) \in \widehat{L}^1$.

Furthermore, recalling that $Q = -V_2\phi \otimes V_1\phi$,

$$\begin{aligned} T_{01}(\lambda) &:= \overline{Q}\widehat{T}(\lambda)Q = \overline{Q}(I + \widehat{T}(\lambda))Q = (I + \widehat{T}(\lambda))Q - Q(I + \widehat{T}(\lambda))Q \\ &= -\big(V_2\big(R_0((\lambda + i0)^2) - R_0(0)\big)V\phi + \lambda c_0(\lambda)V_2\phi\big) \otimes V_1\phi \\ &= -\lambda\bigg(V_2\frac{R_0((\lambda + i0)^2) - R_0(0)}{\lambda}V\phi + c_0(\lambda)V_2\phi\bigg) \otimes V_1\phi. \end{aligned} \tag{2-18}$$

Likewise,

$$\begin{aligned} T_{10}(\lambda) &= -V_2\phi \otimes \big(V_1(R_0^*((\lambda + i0)^2) - R_0(0))V\phi + \lambda\overline{c_0(\lambda)}V_1\phi\big) \\ &= -\lambda V_2\phi \otimes \bigg(V_1\frac{R_0^*((\lambda + i0)^2) - R_0(0)}{\lambda}V\phi + \overline{c_0(\lambda)}V_1\phi\bigg). \end{aligned} \tag{2-19}$$

Thus $T_{10}^\vee$ and $T_{01}^\vee$ are both in $\mathcal{V}_{L^{3/2,2}} \cap \mathcal{V}_{L^{3,2}}$ — $T_{10}^\vee$ by the second line of (2-18) and $T_{01}^\vee$ by the first line of (2-19) — when $V \in L^{\frac{3}{2},1}$. Indeed, following the definition, this reduces to

$$\int_{\mathbb{R}^3} \frac{|V_2(x)||V(y)||\phi(y)|}{4\pi|x-y|}\,dy \in L_x^{\frac{3}{2},2} \cap L_x^{3,2}.$$

Next, $-T_{10}(\lambda)T_{00}^{-1}(\lambda)T_{01}(\lambda) = \lambda c_1(\lambda)Q$, where

$$c_1(\lambda) = -\Big\langle V_1\big(R_0^*((\lambda+i0)^2) - R_0(0)\big)V\phi + \lambda\overline{c_0(\lambda)}V_1\phi,\\ T_{00}^{-1}(\lambda)\Big(V_2\frac{R_0((\lambda+i0)^2) - R_0(0)}{\lambda}V\phi + c_0(\lambda)V_2\phi\Big)\Big\rangle. \quad (2\text{-}20)$$

For example, one term from formula (2-20) has the form

$$\Big\langle V_1\big(R_0^*((\lambda+i0)^2) - R_0(0)\big)V_2V_1\phi,\, T_{00}^{-1}(\lambda)V_2\frac{R_0((\lambda+i0)^2) - R_0(0)}{\lambda}V_1V_2\phi\Big\rangle. \quad (2\text{-}21)$$

Note that $V_1\big(R_0^*((\lambda+i0)^2) - R_0(0)\big)V_2$ and $\chi\big(\frac{\lambda}{\epsilon}\big)T_{00}^{-1}(\lambda)$ are in $\mathcal{W}$, while

$$M\Big(V_2\frac{R_0((\lambda+i0)^2) - R_0(0)}{\lambda}V_1\Big) = \frac{|V_2|\otimes|V_1|}{4\pi} \in \mathcal{B}(L^{\frac{3}{2},2}, L^{3,2}),$$

so

$$V_2\frac{R_0((\lambda+i0)^2) - R_0(0)}{\lambda}V_1 \in \mathcal{V}_{L^{3/2,2},L^{3,2}}.$$

Taking into account the fact that $V_1\phi$, $V_2\phi \in L^{\frac{3}{2},2}$, it follows that (2-21) is in $\widehat{L}^1$.

Thus we recognize from (2-20) that $c_1(\lambda) \in \widehat{L}^1$ when $V \in L^{\frac{3}{2},1}$.

Further note that, since $R_0^*((\lambda+i0)^2) - R_0(0) = 0$ when $\lambda = 0$, we have $c_1(0) = 0$.

Let

$$C(\lambda) := T_{11}(\lambda) - T_{10}(\lambda)T_{00}^{-1}(\lambda)T_{01}(\lambda).$$

Then

$$C(\lambda) = \lambda(c_0(\lambda) + c_1(\lambda))Q.$$

Thus $C(\lambda)/\lambda$ is invertible for $|\lambda| \ll 1$ and $C^{-1}(\lambda) = \lambda^{-1}c_2(\lambda)Q$, with c_2 locally in $\widehat{L}^1$. Consequently, for small ϵ, we have $\big(\chi\big(\frac{\lambda}{\epsilon}\big)\lambda C^{-1}(\lambda)\big)^\vee \in \mathcal{V}_{L^{3,2},L^{3/2,2}}$.

The inverse of $I + \widehat{T}(\lambda)$ is then given for small λ by formula (2-13):

$$(I+\widehat{T})^{-1} = \begin{pmatrix} T_{00}^{-1} + T_{00}^{-1}T_{01}C^{-1}T_{10}T_{00}^{-1} & -T_{00}^{-1}T_{01}C^{-1} \\ -C^{-1}T_{10}T_{00}^{-1} & C^{-1} \end{pmatrix}.$$

Since $T_{00}^{-1} \in \mathcal{W}$ and $T_{01}^\vee, T_{10}^\vee \in \mathcal{V}_{L^{3/2,2}} \cap \mathcal{V}_{L^{3,2}}$, while

$$\Big(\chi\Big(\frac{\lambda}{\epsilon}\Big)\lambda C^{-1}(\lambda)\Big)^\vee \in \mathcal{V}_{L^{3,2},L^{3/2,2}},$$

it immediately follows that

$$\lambda((I+\widehat{T}(\lambda))^{-1} - T_{00}^{-1}(\lambda)) \in \mathcal{V}_{L^{3,2},L^{3/2,2}}$$

and that $(I+\widehat{T})^{-1}$, given by formula (2-13), exists on a whole cut neighborhood of zero. □

Recall that by (1-2)

$$R(t) := \frac{ae^{-i\frac{3\pi}{4}}}{\sqrt{i\pi t}} \zeta_t(x) \otimes \zeta_t(y), \quad \zeta_t(x) := e^{i\frac{|x|^2}{4t}} \phi(x).$$

Proposition 2.13. *Assume that $\langle x\rangle^2 V \in L^{\frac{3}{2},1}$ and that $H = -\Delta + V$ is an exceptional Hamiltonian of the first kind with canonical resonance ϕ at zero. Then, for $1 \leq p < \frac{3}{2}$ and $R(t)$ as above,*

$$e^{-itH} P_c u = Z(t)u + R(t)u,$$

$$\|Z(t)u\|_{L^{p'}} \lesssim t^{-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{p'}\right)} \|f\|_{L^p}, \quad \|Z(t)u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}} \|f\|_{L^{3/2,1}}.$$

Furthermore, for $\frac{3}{2} < p \leq 2$,

$$\|e^{-itH} P_c u\|_{L^{p'}} \lesssim t^{-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{p'}\right)} \|u\|_{L^p}.$$

Here $\frac{1}{p} + \frac{1}{p'} = 1$.

Proof of Proposition 2.13. Write the evolution as

$$e^{-itH} P_c f = \frac{1}{i\pi} \int_{\mathbb{R}} e^{-it\lambda^2} \big(R_0((\lambda+i0)^2) - R_0((\lambda+i0)^2) V_1 \widehat{T}(\lambda)^{-1} V_2 R_0((\lambda+i0)^2)\big) f \lambda \, d\lambda.$$

We consider a partition of unity subordinated to the neighborhoods of Lemmas 2.8 and 2.11. First, take a sufficiently large R such that $\big(1-\chi\big(\frac{\lambda}{R}\big)\big)(I+\widehat{T}(\lambda))^{-1} \in \mathcal{W}$. Then for every $\lambda_0 \in [-4R, 4R]$ there exists $\epsilon(\lambda_0) > 0$ such that

$$\chi\left(\frac{\lambda-\lambda_0}{\epsilon(\lambda_0)}\right)(I+\widehat{T}(\lambda))^{-1} \in \mathcal{W}$$

if $\lambda_0 \neq 0$, while the conclusion of Lemma 2.11 holds when $\lambda_0 = 0$.

Since $[-4R, 4R]$ is a compact set, there exists a finite covering

$$[-4R, 4R] \subset \bigcup_{k=1}^{N} \big(\lambda_k - \epsilon(\lambda_k), \lambda_k + \epsilon(\lambda_k)\big).$$

Then we construct a finite partition of unity on $\mathbb{R}$ by smooth functions $1 = \chi_0(\lambda) + \sum_{k=1}^N \chi_k(\lambda) + \chi_\infty(\lambda)$, where $\operatorname{supp} \chi_\infty \subset \mathbb{R} \setminus (-2R, 2R)$, $\operatorname{supp} \chi_0 \subset [-\epsilon(0), \epsilon(0)]$, and $\operatorname{supp} \chi_k \subset \big[\lambda_k - \epsilon(\lambda_k), \lambda_k + \epsilon(\lambda_k)\big]$.

By Lemma 2.8, for any $k \neq 0$, we have $\chi_k(\lambda)(I+\widehat{T}(\lambda))^{-1} \in \mathcal{W}$, so $(1-\chi_0(\lambda))(I+\widehat{T}(\lambda))^{-1} \in \mathcal{W}$. By Lemma 2.11, $\chi_0(\lambda)\widehat{T}(\lambda)$ also decomposes into a regular term $L \in \mathcal{W}$ and a singular term $-\lambda^{-1}\chi_0(\lambda) a V_2\phi \otimes V_1\phi$.

Let Z_1 be given by the sum of all the regular terms in the decomposition:

$$\begin{aligned} Z_1(t) :=& \frac{1}{i\pi} \int_{\mathbb{R}} e^{-it\lambda^2} \big(R_0((\lambda+i0)^2) - R_0((\lambda+i0)^2) V_1 L(\lambda) V_2 R_0((\lambda+i0)^2) \\ &\qquad - (1-\chi_0(\lambda)) R_0((\lambda+i0)^2) V_1 \widehat{T}(\lambda) V_2 R_0((\lambda+i0)^2)\big) \lambda \, d\lambda \\ =& \frac{1}{2\pi t} \int_{\mathbb{R}} e^{-it\lambda^2} \partial_\lambda \big(R_0((\lambda+i0)^2) - R_0((\lambda+i0)^2) V_1 L(\lambda) V_2 R_0((\lambda+i0)^2) \\ &\qquad - (1-\chi_0(\lambda)) R_0((\lambda+i0)^2) V_1 \widehat{T}(\lambda) V_2 R_0((\lambda+i0)^2)\big) \, d\lambda \end{aligned}$$

$$= \frac{C}{t^{\frac{3}{2}}} \int_{\mathbb{R}} e^{-i\frac{\rho^2}{4t}} \big(\partial_\lambda \big(R_0((\lambda+i0)^2) - R_0((\lambda+i0)^2) V_1 L(\lambda) V_2 R_0((\lambda+i0)^2) \\ -(1-\chi_0(\lambda)) R_0((\lambda+i0)^2) V_1 \widehat{T}(\lambda) V_2 R_0((\lambda+i0)^2)\big)\big)^{\vee}(\rho)\, d\rho.$$

The fact that $\|Z_1(t)u\|_{L^\infty} \lesssim |t|^{-\frac{3}{2}} \|u\|_{L^1}$ follows by knowing that

$$\big(\partial_\lambda \big(R_0((\lambda+i0)^2) - R_0((\lambda+i0)^2) V_1 L(\lambda) V_2 R_0((\lambda+i0)^2) \\ -(1-\chi_0(\lambda)) R_0((\lambda+i0)^2) V_1 \widehat{T}(\lambda) V_2 R_0((\lambda+i0)^2)\big)\big)^{\vee} \in \mathcal{V}_{L^1, L^\infty}.$$

The fact that $\|Z_1(t)u\|_{L^2} \lesssim \|u\|_{L^2}$ follows by smoothing estimates. Indeed, the first term is bounded since it represents the free evolution, and note that

$$\|V_2 R_0(\lambda \pm i0) f\|_{L^2_{\lambda,x}} \lesssim \|f\|_{L^2_x},$$
$$\big\|e^{-it\lambda}(L(\pm\sqrt{\lambda}) + (1-\chi_0(\pm\sqrt{\lambda}))\widehat{T}(\pm\sqrt{\lambda}))\big\|_{L^\infty_\lambda \mathcal{B}(L^2)} < \infty,$$
$$\Big\|\int_{\mathbb{R}} R_0(\lambda \pm i0) V_1 F(x,\lambda)\, d\lambda\Big\|_{L^2_x} \lesssim \|F\|_{L^2_{\lambda,x}}.$$

Combining these three estimates, we obtain the L^2 boundedness of Z_1.

By interpolation between the two bounds, we obtain that, for $\frac{1}{p} + \frac{1}{p'} = 1$, with $1 \le p \le 2$,

$$\|Z_1(t)u\|_{L^{p'}} \lesssim t^{-\frac{3}{2}\left(\frac{1}{p} - \frac{1}{p'}\right)} \|u\|_{L^p},$$

as well as

$$\|Z_1(t)u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}} \|u\|_{L^{3/2,1}}.$$

Let Z_2 be the term corresponding to the singular part of the decomposition from Lemma 2.11, given by

$$Z_2(t) := \frac{a}{i\pi} \int_{\mathbb{R}} e^{-it\lambda^2} \chi_0(\lambda) R_0((\lambda+i0)^2) V\phi \otimes V\phi R_0((\lambda+i0)^2)\, d\lambda \\ = \frac{a}{i\pi} \int_{\mathbb{R}} \int_{(\mathbb{R}^3)^2} e^{-it\lambda^2} \chi_0(\lambda) \frac{e^{i\lambda|x-z_1|}}{4\pi|x-z_1|} V(z_1)\phi(z_1) V(z_2)\phi(z_2) \frac{e^{i\lambda|z_2-y|}}{4\pi|z_2-y|}\, dz_1\, dz_2\, d\lambda.$$

The subsequent Lemma 2.14 is the same as [Yajima 2005, Lemma 4.10], the only difference being the space of potentials for which the result holds. For the sake of completeness, we repeat the proof given in [Yajima 2005].

Lemma 2.14. *For $V \in \langle x\rangle^{-1} L^{\frac{3}{2},1}$,*

$$\|(Z_2(t) - R(t))u\|_{L^\infty} \lesssim t^{-\frac{3}{2}} \|u\|_{L^1}, \quad \|Z_2(t)u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}} \|u\|_{L^{3/2,1}}. \tag{2-22}$$

Proof of Lemma 2.14. Let $b = |x - z_1| + |z_2 - y|$ and

$$C(t,b) = \frac{1}{i\pi} \int_{\mathbb{R}} e^{-it\lambda^2 + i\lambda b} \chi_0(\lambda)\, d\lambda.$$

We express $Z_2(t)$ as

$$Z_2(t) = \int_{(\mathbb{R}^3)^2} C(t,b)a \frac{V(z_1)\phi(z_1)V(z_2)\phi(z_2)}{|x-z_1|\,|z_2-y|}\,dz_1\,dz_2.$$

Note that

$$C(t,b) = \frac{e^{-i\frac{3\pi}{4}}e^{i\frac{b^2}{4t}}}{\sqrt{\pi t}}\big(e^{i\frac{s^2}{4t}}\chi_0^\vee(s)\big)^\wedge\Big(\frac{b}{2t}\Big).$$

Then $C(t,b) \lesssim t^{-\frac{1}{2}}$ and

$$|Z_2(t)(x,y)| \lesssim t^{-\frac{1}{2}} \int_{(\mathbb{R}^3)^2} \frac{|V(z_1)\phi(z_1)V(z_2)\phi(z_2)|}{|z_1-x|\,|z_2-y|}\,dz_1\,dz_2.$$

Clearly

$$\int_{\mathbb{R}^3} \frac{|V(z_1)\phi(z_1)|}{|z_1-x|}\,dz_1 \in L^{3,\infty}_x \quad \text{and} \quad \int_{\mathbb{R}^3} \frac{|V(z_2)\phi(z_2)|}{|z_2-y|}\,dz_2 \in L^{3,\infty}_y,$$

implying the second half of (2-22):

$$\|Z_2(t)u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}}\|u\|_{L^{3/2,1}}.$$

We also have

$$\Big|\mathcal{F}(e^{\frac{is^2}{4t}}\chi_0^\vee(s))\Big(\frac{b}{2t}\Big)-1\Big| \lesssim t^{-1}\big(\|s^2\chi_0^\vee\|_1+|b|\big).$$

It is easy to see, for

$$B = 2\big(|x-z_1|\,|z_1|+|z_2-y|\,|z_2|+|x-z_1|\,|z_2-y|\big)+|z_1|^2+|z_2|^2,$$

that

$$|e^{ib^2/4t}-e^{i(x^2+y^2)/4t}| = \big|e^{i(|x-z_1|+|z_2-y|)^2/4t}-e^{i(x^2+y^2)/4t}\big| \le \frac{B}{4t}.$$

It follows that

$$C(t,b) - \frac{e^{-i\frac{3\pi}{4}}e^{i(x^2+y^2)/4t}}{\sqrt{\pi t}} \lesssim (1+b+B)t^{-\frac{3}{2}}.$$

Then

$$\Big|Z_2(t) - \int_{(\mathbb{R}^3)^2} \frac{e^{i\frac{3\pi}{4}}e^{i(x^2+y^2)/4t}}{\sqrt{\pi t}} a \frac{V(z_1)\phi(z_1)V(z_2)\phi(z_2)\,dz_1\,dz_2}{|x-z_1|\,|y-z_2|}\Big| \\ \lesssim t^{-\frac{3}{2}} \int_{(\mathbb{R}^3)^2} \frac{(1+b+B)\big|V(z_1)\phi(z_1)V(z_2)\phi(z_2)\big|}{|x-z_1|\,|z_2-y|}\,dz_1\,dz_2.$$

Now note that, for $V \in \langle x\rangle^{-1}L^{\frac{3}{2},1}$ and $\phi(x) \lesssim |x|^{-1}$,

$$\sup_{x,y} \int_{(\mathbb{R}^3)^2} \frac{(1+b+B)|V(z_1)\phi(z_1)V(z_2)\phi(z_2)|}{|x-z_1|\,|z_2-y|}\,dz_1\,dz_2 < \infty$$

and

$$\int_{\mathbb{R}^3} \frac{V(z_1)\phi(z_1)\,dz_1}{|x-z_1|} = \phi(x).$$

The first part of conclusion (2-22) follows. □

Note that $R(t)$ also satisfies $\|R(t)u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}}\|u\|_{L^{3/2,1}}$, so the same holds for the difference:

$$\|(Z_2(t)-R(t))u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}}\|u\|_{L^{3/2,1}}.$$

By interpolation with the L^1-to-L^∞ estimate of Lemma 2.14, we obtain that, for $1 \le p < \frac{3}{2}$,

$$\|(Z_2(t)-R(t))u\|_{L^{p'}} \lesssim t^{-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{p'}\right)}\|u\|_{L^p}.$$

Since the same is true for Z_1, we obtain for $1 \le p < \frac{3}{2}$ that

$$\|(Z(t)u\|_{L^{p'}} = \left\|(Z_1(t)+Z_2(t)-R(t))u\right\|_{L^{p'}} \lesssim t^{-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{p'}\right)}\|u\|_{L^p},$$

where $e^{-itH}P_c u = Z_1(t)u + Z_2(t)u = Z(t)u + R(t)u$.

Knowing that $\|Z_i(t)u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}}\|u\|_{L^{3/2,1}}$ leads to the conclusion that $\|e^{-itH}P_c u\|_{L^{3,\infty}} \lesssim \|u\|_{L^{3/2,1}}$. Combining this with the L^2 estimate $\|e^{-itH}P_c u\|_{L^2} \lesssim \|u\|_{L^2}$, we obtain that, for $\frac{3}{2} < p \le 2$,

$$\|e^{-itH}P_c u\|_{L^{p'}} \lesssim t^{-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{p'}\right)}\|u\|_{L^p}.$$

Thus we have proved all the conclusions of Proposition 2.13. □

Proposition 2.15. *Assume that $V \in L^{\frac{3}{2},1}$ and that $H = -\Delta + V$ is an exceptional Hamiltonian of the first kind. Then*

$$\|e^{-itH}P_c u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}}\|u\|_{L^{3/2,1}},$$

and, for $\frac{3}{2} < p \le 2$,

$$\|e^{-itH}P_c u\|_{L^{p'}} \lesssim t^{-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{p'}\right)}\|u\|_{L^p}.$$

Here $\frac{1}{p}+\frac{1}{p'}=1$.

Proof of Proposition 2.15. Write the evolution as

$$e^{-itH}P_c f = \frac{1}{i\pi}\int_{\mathbb{R}} e^{-it\lambda^2}\big(R_0((\lambda+i0)^2) - R_0((\lambda+i0)^2)V_1\widehat{T}(\lambda)^{-1}V_2R_0((\lambda+i0)^2)\big)f\lambda\,d\lambda.$$

We consider a partition of unity subordinated to the neighborhoods of Lemmas 2.8 and 2.12. First, take a sufficiently large R such that $\big(1-\chi\big(\frac{\lambda}{R}\big)\big)(I+\widehat{T}(\lambda))^{-1} \in \mathcal{W}$. Then, for every $\lambda_0 \in [-4R, 4R]$, there exists $\epsilon(\lambda_0) > 0$ such that

$$\chi\left(\frac{\lambda-\lambda_0}{\epsilon(\lambda_0)}\right)(I+\widehat{T}(\lambda))^{-1} \in \mathcal{W}$$

if $\lambda_0 \neq 0$, while the conclusion of Lemma 2.12 holds when $\lambda_0 = 0$.

Since $[-4R, 4R]$ is a compact set, there exists a finite covering

$$[-4R, 4R] \subset \bigcup_{k=1}^{N}\big(\lambda_k - \epsilon(\lambda_k), \lambda_k + \epsilon(\lambda_k)\big).$$

Then we construct a finite partition of unity on $\mathbb{R}$ by smooth functions $1 = \chi_0(\lambda) + \sum_{k=1}^{N}\chi_k(\lambda) + \chi_\infty(\lambda)$, where $\operatorname{supp}\chi_\infty \subset \mathbb{R}\setminus(-2R, 2R)$, $\operatorname{supp}\chi_0 \subset [-\epsilon(0), \epsilon(0)]$, and $\operatorname{supp}\chi_k \subset \big[\lambda_k - \epsilon(\lambda_k), \lambda_k + \epsilon(\lambda_k)\big]$.

By Lemma 2.8, for any $k \neq 0$, we have $\chi_k(\lambda)(I+\widehat{T}(\lambda))^{-1} \in \mathcal{W}$, so $(1-\chi_0(\lambda))(I+\widehat{T}(\lambda))^{-1} \in \mathcal{W}$. By Lemma 2.12, $\chi_0(\lambda)(I+\widehat{T}(\lambda))^{-1}$ also decomposes into a regular term $L \in \mathcal{W}$ and a singular term $\lambda^{-1}S$, with the property that $S^\vee \in \mathcal{V}_{L^{3,2},L^{3/2,2}}$.

Let Z_1 be given by the sum of all the regular terms of the decomposition:

$$\begin{aligned} Z_1(t) :=& \frac{1}{i\pi}\int_{\mathbb{R}} e^{-it\lambda^2}\big(R_0((\lambda+i0)^2)-R_0((\lambda+i0)^2)V_1L(\lambda)V_2R_0((\lambda+i0)^2) \\ &\qquad -(1-\chi_0(\lambda))R_0((\lambda+i0)^2)V_1\widehat{T}(\lambda)V_2R_0((\lambda+i0)^2)\big)\lambda\,d\lambda \\ =& \frac{1}{2\pi t}\int_{\mathbb{R}} e^{-it\lambda^2}\partial_\lambda\big(R_0((\lambda+i0)^2)-R_0((\lambda+i0)^2)V_1L(\lambda)V_2R_0((\lambda+i0)^2) \\ &\qquad -(1-\chi_0(\lambda))R_0((\lambda+i0)^2)V_1\widehat{T}(\lambda)V_2R_0((\lambda+i0)^2)\big)\,d\lambda \\ =& \frac{C}{t^{\frac{3}{2}}}\int_{\mathbb{R}} e^{-i\frac{\rho^2}{4t}}\big(\partial_\lambda\big(R_0((\lambda+i0)^2)-R_0((\lambda+i0)^2)V_1L(\lambda)V_2R_0((\lambda+i0)^2) \\ &\qquad -(1-\chi_0(\lambda))R_0((\lambda+i0)^2)V_1\widehat{T}(\lambda)V_2R_0((\lambda+i0)^2)\big)\big)^\vee(\rho)\,d\rho. \end{aligned}$$

The fact that $\|Z_1(t)u\|_{L^\infty} \lesssim |t|^{-\frac{3}{2}}\|u\|_{L^1}$ follows by knowing that

$$\begin{aligned} &\big(\partial_\lambda\big(R_0((\lambda+i0)^2)-R_0((\lambda+i0)^2)V_1L(\lambda)V_2R_0((\lambda+i0)^2) \\ &\qquad -(1-\chi_0(\lambda))R_0((\lambda+i0)^2)V_1\widehat{T}(\lambda)V_2R_0((\lambda+i0)^2)\big)\big)^\vee \in \mathcal{V}_{L^1,L^\infty}. \end{aligned}$$

Using smoothing estimates, it immediately follows that $Z_1(t)$ is L^2-bounded; see the proof of Proposition 2.13. Interpolating, we obtain the desired $\|Z_1(t)u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}}\|u\|_{L^{3,1}}$ estimate.

Let Z_2 be the singular part of the decomposition from Lemma 2.12, given by

$$Z_2(t) := \frac{1}{i\pi}\int_{\mathbb{R}} e^{-it\lambda^2}R_0((\lambda+i0)^2)V_1S(\lambda)V_2R_0((\lambda+i0)^2)\,d\lambda. \tag{2-23}$$

Note that $\big(R_0((\lambda+i0)^2)V_1\big)^\vee \in \mathcal{V}_{L^{3/2,2},L^{3,\infty}}$, $S(\lambda)^\vee \in \mathcal{V}_{L^{3,2},L^{3/2,2}}$, and $\big(V_2R_0((\lambda+i0)^2)\big)^\vee \in \mathcal{V}_{L^{3/2,1},L^{3,2}}$. Thus

$$R_0((\lambda+i0)^2)V_1(\lambda S(\lambda))V_2R_0((\lambda+i0)^2) \in \mathcal{V}_{L^{3/2,1},L^{3,\infty}}.$$

By taking the Fourier transform in (2-23), this immediately implies the conclusion that $\|Z_2(t)u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}}\|u\|_{L^{3/2,1}}$.

Putting the two estimates for Z_1 and Z_2 together, we obtain that $\|e^{-itH}P_cu\|_{L^{3,\infty}} \lesssim \|u\|_{L^{3/2,1}}$. Interpolating with the obvious L^2 bound $\|e^{-itH}P_cu\|_{L^2} \lesssim \|u\|_{L^2}$, we obtain the stated conclusion. □

2F. ***Exceptional Hamiltonians of the third kind.*** We next consider the case in which H is exceptional of the third kind; that is, there are both zero eigenvectors and zero resonances. Recall that $\widehat{T}(\lambda) = V_2R_0((\lambda+i0)^2)V_1$.

Lemma 2.16. *Suppose that $V \in \langle x\rangle^{-4}L^{\frac{3}{2},1}$ and $H = -\Delta + V$ has both eigenvectors and resonances at zero. Let χ be a standard cutoff function. Then, for sufficiently small ϵ,*

$$\chi\Big(\frac{\lambda}{\epsilon}\Big)(I+\widehat{T}(\lambda))^{-1} = L(\lambda) + \chi\Big(\frac{\lambda}{\epsilon}\Big)\Big(\frac{V_2P_0V_1}{\lambda^2} + \frac{iV_2P_0V|x-y|^2VP_0V_1}{\lambda} - \frac{aV_2\phi\otimes V_1\phi}{\lambda}\Big),$$

where $L(\lambda) \in \mathcal{W}$ *and* ϕ *is a certain resonance for* $H = -\Delta + V$.

Furthermore, 0 *is an isolated exceptional point for* H, *meaning that* H *has finitely many negative eigenvalues.*

The computations in the proof of this lemma parallel those in [Yajima 2005, Section 4.5]. The main difference is in using the space $\mathcal{W}$ instead of Hölder spaces.

Proof of Lemma 2.16. We study $(I + \widehat{T}(\lambda))^{-1} := \big(I + V_2 R_0((\lambda + i0)^2) V_1\big)^{-1}$ near $\lambda = 0$.

Let

$$Q = -\frac{1}{2\pi i} \int_{|z+1|=\delta} \big(V_2 R_0(0) V_1 - zI\big)^{-1}\, dz.$$

Take the orthonormal basis $\{\phi_1, \dots, \phi_N\}$ with respect to the inner product $-(Vu, v)$ for $\mathcal{M}$ so that $\{\phi_2, \dots, \phi_N\}$ is a basis of $\mathcal{E}$ and $\langle \phi_1, V\rangle > 0$. This condition determines ϕ_1 uniquely.

Define the orthogonal projections π_1 onto $\mathbb{C} V_1 \phi_1$ and π_2 onto $V_1 P_0 L^2$ with respect to the inner product $-(\operatorname{sgn} V u, v)$, i.e., $\pi_1 = -V_2\phi_1 \otimes V_1 \phi_1$ and $\pi_2 = -\sum_{j=2}^N V_2 \phi_j \otimes V_1 \phi_j$, and let

$$Q_0 = \overline{Q} := 1 - Q, \quad Q_1 := Q\pi_1 Q, \quad Q_2 := Q \pi_2 Q.$$

The following identities hold in L^2:

$$\begin{gathered}
Q_j Q_k = \delta_{jk} I \quad \text{for } j, k = 0, 1, 2, \qquad Q_0 + Q_1 + Q_2 = I,\\
\big(I + V_2 R_0(0) V_1\big) Q_1 = Q_1 \big(I + V_2 R_0(0) V_1\big) = 0,\\
\big(I + V_2 R_0(0) V_1\big) Q_2 = Q_2 \big(I + V_2 R_0(0) V_1\big) = 0,\\
Q_2(V_2 \otimes V_1) Q_0 = 0, \quad Q_2(V_2 \otimes V_1) Q_1 = 0, \quad Q_2 (V_2 \otimes V_1) Q_2 = 0,\\
Q_0 (V_2 \otimes V_1) Q_2 = 0, \quad Q_1 (V_2 \otimes V_1) Q_2 = 0.
\end{gathered}$$

These identities follow from $Q_2 V_2 = 0$ and $Q_2^* V_1 = 0$, which in turn follow from the fact that eigenvectors ϕ_k are orthogonal to V, that is, $\langle \phi_k, V\rangle = 0$ for $2 \le k \le N$.

We first apply Lemma 2.10 to invert $Q(I + \widehat{T}(\lambda))Q$ in QL^2 for small λ, after writing it in matrix form with respect to the decomposition $QL^2 = Q_1 L^2 + Q_2 L^2$:

$$Q(I + \widehat{T}(\lambda))Q = \begin{pmatrix} Q_1 (I + \widehat{T}(\lambda)) Q_1 & Q_1 \widehat{T}(\lambda) Q_2 \\ Q_2 \widehat{T}(\lambda) Q_1 & Q_2 (I + \widehat{T}(\lambda)) Q_2 \end{pmatrix} =: \begin{pmatrix} T_{11}(\lambda) & T_{12}(\lambda) \\ T_{21}(\lambda) & T_{22}(\lambda) \end{pmatrix}.$$

The inverse will be given by formula (2-13); that is,

$$\big(Q(I + \widehat{T}(\lambda))Q\big)^{-1} = \begin{pmatrix} T_{11}^{-1} + T_{11}^{-1} T_{12} C_{22}^{-1} T_{21} T_{11}^{-1} & -T_{11}^{-1} T_{12} C_{22}^{-1} \\ -C_{22}^{-1} T_{21} T_{11}^{-1} & C_{22}^{-1} \end{pmatrix}, \tag{2-24}$$

where

$$C_{22} = T_{22} - T_{21} T_{11}^{-1} T_{12}.$$

As in the case of exceptional Hamiltonians of the first kind, let

$$J(\lambda) := \frac{\widehat{T}(\lambda) - \big(V_2 R_0(0) V_1 + i\lambda (4\pi)^{-1} V_2 \otimes V_1\big)}{\lambda^2}.$$

Then (recall that $Q_1 = -V_2\phi_1 \otimes V_1\phi_1$),

$$\begin{aligned} T_{11}(\lambda) &= Q_1(I + \widehat{T}(\lambda))Q_1 = Q_1\big(I + V_2 R_0((\lambda+i0)^2)V_1\big)Q_1 \\ &= Q_1\big(V_2 R_0((\lambda+i0)^2)V_1 - V_2 R_0(0)V_1\big)Q_1 \\ &= V_2\phi_1 \otimes V\phi_1\big(R_0((\lambda+i0)^2) - R_0(0)\big)V\phi_1 \otimes V_1\phi_1 \\ &= \left(\lambda\frac{|\langle V,\phi_1\rangle|^2}{4i\pi} - \lambda^2\langle V_1\phi_1, J(\lambda)V_2\phi_1\rangle\right)Q_1 \\ &=: (\lambda a^{-1} + \lambda^2 c_1(\lambda))Q_1. \end{aligned}$$

Here $a = 4i\pi/|\langle V,\phi_1\rangle|^2 \neq 0$. As in the proof of Lemma 2.11, note that $c_1(\lambda) \in \widehat{L}^1$ when $V \in L^1$ and $\partial_\lambda c_1(\lambda) \in \widehat{L}^1$ when $V \in \langle x\rangle^{-1}L^1$.

It follows that $T_{11}(\lambda)$ is invertible for $|\lambda| \ll 1$ in $Q_1 L^2$ and

$$\begin{aligned} T_{11}^{-1}(\lambda) &= \frac{1}{\lambda a^{-1} + \lambda^2 c_1(\lambda)}Q_1 \\ &= \left(\frac{a}{\lambda} - \frac{c_1(\lambda)}{(a^{-1} + \lambda c_1(\lambda))a^{-1}}\right)Q_1 \\ &= \lambda^{-1}aQ_1 + E(\lambda). \end{aligned}$$

Here and below we denote various regular terms by $E(\lambda)$, i.e., terms with the property that $\chi\big(\frac{\lambda}{\epsilon}\big)E(\lambda) \in \mathcal{W}$ for sufficiently small ϵ.

Likewise, since $Q_2(V_2 \otimes V_1) = (V_2 \otimes V_1)Q_2 = 0$,

$$\begin{aligned} T_{12}(\lambda) &= Q_1\big(I + V_2 R_0((\lambda+i0)^2)V_1\big)Q_2 \\ &= Q_1 V_2\left(R_0((\lambda+i0)^2) - R_0(0) - i\lambda\frac{1\otimes 1}{4\pi}\right)V_1 Q_2 \\ &= -\lambda^2 Q_1\left(V_2\frac{|x-y|}{8\pi}V_1 + \lambda V_2 e_1(\lambda)V_1\right)Q_2 \\ &= -\lambda^2 Q_1 V_2\frac{|x-y|}{8\pi}V_1 Q_2 + \lambda^3 E(\lambda), \end{aligned}$$

where

$$e_1(\lambda) := \frac{R_0((\lambda+i0)^2) - R_0(0) - i\lambda\frac{1\otimes 1}{4\pi} + \lambda^2\frac{|x-y|}{8\pi}}{-\lambda^3}.$$

By Lemma 2.6,

$$M((e_1(\lambda))^\wedge) = \frac{|x-y|^2}{24\pi} \quad \text{and} \quad M((\partial_\lambda e_1(\lambda))^\wedge) = \frac{|x-y|^3}{96\pi}.$$

Thus $E(\lambda) := Q_1 V_2 e_1(\lambda) V_1 Q_2 \in \mathcal{W}$ when

$$\int_{(\mathbb{R}^3)^2} V(x)\phi_1(x)|x-y|^3 V(y)\phi_k(y)\,dx\,dy < \infty,$$

which takes place when $V \in \langle x\rangle^{-2}L^1$ (recall that $|\phi_1(y)| \lesssim \langle y\rangle^{-1}$).

Likewise we obtain

$$T_{21}(\lambda) = -\lambda^2 Q_2 V_2 \frac{|x-y|}{8\pi} V_1 Q_1 + \lambda^3 E(\lambda);$$

hence, combining the previous results,

$$T_{21}(\lambda) T_{11}^{-1}(\lambda) T_{12}(\lambda) = \lambda^3 a Q_2 V_2 \frac{|x-y|}{8\pi} V_1 Q_1 V_2 \frac{|x-y|}{8\pi} V_1 Q_2 + E(\lambda).$$

Furthermore,

$$\begin{aligned} T_{22}(\lambda) &= Q_2\big(I + V_2 R_0((\lambda+i0)^2) V_1\big) Q_2 \\ &= Q_2 V_2 \Big(R_0((\lambda+i0)^2) - R_0(0) - i\lambda \frac{1\otimes 1}{4\pi}\Big) V_1 Q_2 \\ &= -\lambda^2 Q_2 \Big(V_2 \frac{|x-y|}{8\pi} V_1 + i\lambda V_2 \frac{|x-y|^2}{24\pi} V_1 - \lambda^2 V_2 e_2(\lambda) V_1 \Big) Q_2. \end{aligned}$$

Here

$$e_2(\lambda) := \lambda^{-4}\Big(R_0((\lambda+i0)^2) - R_0(0) - i\lambda \frac{1\otimes 1}{4\pi} - i\lambda^2 \frac{|x-y|}{8\pi} - \lambda^3 \frac{|x-y|^2}{24\pi}\Big).$$

By Lemma 2.6,

$$M(e_2(\lambda)^\wedge) = \frac{|x-y|^3}{96\pi} \quad \text{and} \quad M((\partial_\lambda e_2(\lambda))^\wedge) = \frac{|x-y|^4}{480\pi}.$$

Thus $E(\lambda) := Q_2 V_2 e_2(\lambda) V_1 Q_2 \in \mathcal{W}$ when

$$\int_{(\mathbb{R}^3)^2} V(x)\phi_k(x)|x-y|^4 V(y)\phi_k(y)\,dx\,dy < \infty,$$

which holds true when $V \in \langle x\rangle^{-2} L^1$ (recall that $|\phi_k(y)| \lesssim \langle y\rangle^{-2}$). Then

$$T_{22}(\lambda) = -\lambda^2 Q_2 \Big(V_2 \frac{|x-y|}{8\pi} V_1 + i\lambda V_2 \frac{|x-y|^2}{24\pi} V_1 \Big) Q_2 + \lambda^4 E(\lambda). \tag{2-25}$$

Let P_0 be the L^2 orthogonal projection onto the set $\mathcal{E}$ spanned by $\phi_2, \dots, \phi_N$. By relation (4.38) of [Yajima 2005],

$$\Big(Q_2 V_2 \frac{|x-y|}{8\pi} V_1 Q_2 \Big)^{-1} = -V_2 P_0 V_1.$$

Also note that

$$V_2 P_0 V_1 Q_2 = Q_2 V_2 P_0 V_1 = V_2 P_0 V_1.$$

By (2-25),

$$\begin{aligned} T_{22}^{-1}(\lambda) = -\lambda^{-2} &\Big(Q_2 V_2 \frac{|x-y|}{8\pi} V_1 Q_2 \Big)^{-1} \\ &\sum_{k=0}^{\infty} (-1)^k \bigg(\Big(i\lambda Q_2 V_2 \frac{|x-y|^2}{24\pi} V_1 Q_2 - \lambda^2 E(\lambda) \Big) \Big(Q_2 V_2 \frac{|x-y|}{8\pi} V_1 Q_2 \Big)^{-1} \bigg)^k \\ = \lambda^{-2} V_2 P_0 V_1 &\sum_{k=0}^{\infty} \Big(i\lambda V_2 \frac{|x-y|^2}{24\pi} V_1 - \lambda^2 E(\lambda) \Big) V_2 P_0 V_1. \end{aligned}$$

Therefore, by grouping the terms by the powers of λ, for $|\lambda| \ll 1$,

$$T_{22}^{-1}(\lambda) = \lambda^{-2} V_2 P_0 V_1 + i\lambda^{-1} V_2 P_0 V \frac{|x-y|^2}{24\pi} V P_0 V_1 + E(\lambda).$$

Then we write

$$\begin{aligned} C_{22}(\lambda) &= T_{22}(\lambda) - T_{21}(\lambda) T_{11}^{-1}(\lambda) T_{12}(\lambda) \\ &= \big(I - T_{21}(\lambda) T_{11}^{-1}(\lambda) T_{12}(\lambda) T_{22}^{-1}(\lambda)\big) T_{22}(\lambda). \end{aligned}$$

By our previous estimates, $T_{21}(\lambda)T_{11}^{-1}(\lambda)T_{12}(\lambda)T_{22}^{-1}(\lambda) = \lambda E(\lambda)$, where $E(\lambda) \in \mathcal{W}$. Then, by means of a Neumann series expansion, we retrieve that

$$\begin{aligned} C_{22}^{-1}(\lambda) &= T_{22}^{-1}(\lambda) \sum_{k=0}^{\infty} \big(T_{21}(\lambda) T_{11}^{-1}(\lambda) T_{12}(\lambda) T_{22}^{-1}(\lambda)\big)^k \\ &= T_{22}^{-1}(\lambda) + T_{22}^{-1}(\lambda) T_{21}(\lambda) T_{11}^{-1}(\lambda) T_{12}(\lambda) T_{22}^{-1}(\lambda) + E(\lambda), \end{aligned}$$

so

$$\begin{aligned} C_{22}^{-1}(\lambda) = \lambda^{-2} V_2 P_0 V_1 + i\lambda^{-1} V_2 P_0 V \frac{|x-y|^2}{24\pi} V P_0 V_1 \\ + a\lambda^{-1} V_2 P_0 V \frac{|x-y|}{8\pi} V_1 Q_1 V_2 \frac{|x-y|}{8\pi} V P_0 V_1 + E(\lambda). \end{aligned}$$

If we set

$$\tilde{\phi}_1 = P_0 V \frac{|x-y|}{8\pi} V \phi_1 \in \mathcal{E},$$

then

$$V_2 P_0 V \frac{|x-y|}{8\pi} V_1 Q_1 V_2 \frac{|x-y|}{8\pi} V P_0 V_1 = -V_2 \tilde{\phi}_1 \otimes \tilde{\phi}_1 V_1.$$

Then we get that

$$C_{22}^{-1}(\lambda) = \lambda^{-2} V_2 P_0 V_1 + i\lambda^{-1} V_2 P_0 V \frac{|x-y|^2}{24\pi} V P_0 V_1 - \lambda^{-1} a V_2 \tilde{\phi}_1 \otimes \tilde{\phi}_1 V_1 + E(\lambda).$$

Furthermore,

$$\begin{aligned} -T_{11}^{-1}(\lambda) T_{12}(\lambda) C_{22}^{-1}(\lambda) &= (\lambda^{-1} a Q_1 + E(\lambda)) \lambda^2 Q_1 \left(V_2 \frac{|x-y|}{8\pi} V_1 + \lambda E(\lambda)\right) Q_2 \big(\lambda^{-2} V_2 P_0 V_1 + i\lambda^{-1} E(\lambda)\big) \\ &= \lambda^{-1} a(-V_2\phi_1 \otimes V_1 \phi_1) V_2 \frac{|x-y|}{8\pi} V P_0 V_1 + E(\lambda) \\ &= -a\lambda^{-1} V_2 \phi_1 \otimes \tilde{\phi}_1 V_1 + E(\lambda). \end{aligned}$$

Likewise we obtain

$$\begin{aligned} -C_{22}^{-1}(\lambda) T_{21}(\lambda) T_{11}^{-1}(\lambda) &= -a\lambda^{-1} V_2 \tilde{\phi}_1 \otimes \phi_1 V_1 + E(\lambda), \\ T_{11}^{-1}(\lambda) T_{12}(\lambda) C_{22}^{-1}(\lambda) T_{21}(\lambda) T_{11}^{-1}(\lambda) &= E(\lambda). \end{aligned}$$

By (2-24), we have that $\big(Q(I + \widehat{T}(\lambda))Q\big)^{-1}$ is given in matrix form modulo $E(\lambda) \in \mathcal{W}$ by

$$\begin{pmatrix} -a\lambda^{-1} V_2 \phi_1 \otimes V_1 \phi_1 & -a\lambda^{-1} V_2 \phi_1 \otimes V_1 \tilde{\phi}_1 \\ -a\lambda^{-1} V_2 \tilde{\phi}_1 \otimes V_1 \phi_1 & \lambda^{-2} V_2 P_0 V_1 + i\lambda^{-1} V_2 P_0 V \frac{|x-y|^2}{24\pi} V P_0 V_1 - \lambda^{-1} a V_2 \tilde{\phi}_1 \otimes V_1 \tilde{\phi}_1 \end{pmatrix}. \tag{2-26}$$

Therefore, if we define the canonical resonance as $\phi = \phi_1 - \tilde{\phi}_1$, we have that ϕ satisfies $\phi \in \mathcal{M}$ and $\langle \phi, V \rangle = 1$ and

$$\big(Q(I + \widehat{T}(\lambda))Q\big)^{-1} = \frac{V_2 P_0 V_1}{\lambda^2} + \frac{i V_2 P_0 V \frac{|x-y|^2}{24\pi} V P_0 V_1}{\lambda} - \frac{a V_2 \phi \otimes V_1 \phi}{\lambda} + E(\lambda). \tag{2-27}$$

We apply Lemma 2.10 again after writing $I + \widehat{T}(\lambda)$ in matrix form with respect to the decomposition $L^2 = \overline{Q}L^2 + QL^2$, where $QL^2 = V_2\mathcal{M}$:

$$I + \widehat{T}(\lambda) = \begin{pmatrix} \overline{Q}(I + \widehat{T}(\lambda))\overline{Q} & \overline{Q}\widehat{T}(\lambda)Q \\ Q\widehat{T}(\lambda)\overline{Q} & Q(I + \widehat{T}(\lambda))Q \end{pmatrix} := \begin{pmatrix} S_{00}(\lambda) & S_{01}(\lambda) \\ S_{10}(\lambda) & S_{11}(\lambda) \end{pmatrix}.$$

Next, let $A(\lambda) := S_{00}(\lambda)^{-1}$. Then $\chi\big(\frac{\lambda}{\epsilon}\big)A(\lambda) \in \mathcal{W}$ for sufficiently small ϵ. Indeed, it is easy to see that $S_{00}(\lambda) \in \mathcal{W}$. Furthermore, $S_{00}(0)$ is invertible on $\overline{Q}L^{\frac{3}{2},2} \cap \overline{Q}L^{3,2}$ of inverse K; see (2-12).

As in the proof of Lemma 2.11, let

$$S_\epsilon(\lambda) = \chi\Big(\frac{\lambda}{\epsilon}\Big)\overline{Q}(\widehat{T}(\lambda) - \widehat{T}(0))\overline{Q}.$$

A simple argument based on condition (C1) shows that $\lim_{\epsilon\to 0} \|S_\epsilon(\lambda)\|_{\mathcal{V}_{L^{3/2,2}} \cap \mathcal{V}_{L^{3,2}}} = 0$. Then

$$\begin{aligned}\chi\Big(\frac{\lambda}{\epsilon}\Big)S_{00}^{-1}(\lambda) &= \chi\Big(\frac{\lambda}{\epsilon}\Big)\Big(S_{00}(0) + \chi\Big(\frac{\lambda}{2\epsilon}\Big)\overline{Q}(\widehat{T}(\lambda) - \widehat{T}(0))\overline{Q}\Big)^{-1} \\ &= \chi\Big(\frac{\lambda}{\epsilon}\Big)S_{00}^{-1}(0)\sum_{k=0}^{\infty}(-1)^k\big(S_{2\epsilon}(\lambda)S_{00}^{-1}(0)\big)^k.\end{aligned}$$

This series converges for sufficiently small ϵ, showing that $\big(\chi\big(\frac{\lambda}{\epsilon}\big)S_{00}^{-1}(\lambda)\big)^\vee \in \mathcal{V}_{L^{3/2,2}} \cap \mathcal{V}_{L^{3,2}}$.

Concerning the derivative,

$$\chi\Big(\frac{\lambda}{\epsilon}\Big)\partial_\lambda S_{00}^{-1}(\lambda) = -\chi\Big(\frac{\lambda}{\epsilon}\Big)S_{00}^{-1}(\lambda)\partial_\lambda S_{00}(\lambda)\chi\Big(\frac{\lambda}{2\epsilon}\Big)S_{00}^{-1}(\lambda).$$

In this expression,

$$\Big(\chi\Big(\frac{\lambda}{\epsilon}\Big)S_{00}^{-1}(\lambda)\Big)^\vee \in \mathcal{V}_{L^{3/2,2}} \cap \mathcal{V}_{L^{3,2}} \quad \text{and} \quad \Big(\chi\Big(\frac{\lambda}{2\epsilon}\Big)\partial_\lambda S_{00}(\lambda)\Big)^\vee \in \mathcal{V}_{L^{3/2,2},L^{3,2}}$$

since $M((\partial_\lambda T_{00}(\lambda))^\vee) = (|V_2| \otimes |V_1|)/(4\pi)$. Thus

$$\Big(\chi\Big(\frac{\lambda}{\epsilon}\Big)\partial_\lambda S_{00}^{-1}(\lambda)\Big)^\vee \in \mathcal{V}_{L^{3/2,2},L^{3,2}}.$$

From this we infer that $\chi\big(\frac{\lambda}{\epsilon}\big)A(\lambda) \in \mathcal{W}$, so A is a regular term.

We compute the inverse of $I + \widehat{T}(\lambda)$ by finding each of its matrix elements:

$$(I + \widehat{T}(\lambda))^{-1} = \begin{pmatrix} A + AS_{01}C^{-1}S_{10}A & AS_{01}C^{-1} \\ -C^{-1}S_{10}A & C^{-1} \end{pmatrix}. \tag{2-28}$$

Here

$$C(\lambda) = S_{11}(\lambda) - S_{10}(\lambda)A(\lambda)S_{01}(\lambda).$$

$S_{10}(\lambda)A(\lambda)S_{01}(\lambda) = Q\widehat{T}(\lambda)A(\lambda)\widehat{T}(\lambda)Q$ may be written as

$$\begin{pmatrix} Q_1\widehat{T}(\lambda)A(\lambda)\widehat{T}(\lambda)Q_1 & Q_1\widehat{T}(\lambda)A(\lambda)\widehat{T}(\lambda)Q_2 \\ Q_2\widehat{T}(\lambda)A(\lambda)\widehat{T}(\lambda)Q_1 & Q_2\widehat{T}(\lambda)A(\lambda)\widehat{T}(\lambda)Q_2 \end{pmatrix} = \begin{pmatrix} \lambda^2 E_{11}(\lambda) & \lambda^3 E_{12}(\lambda) \\ \lambda^3 E_{21}(\lambda) & \lambda^4 E_{22}(\lambda) \end{pmatrix}. \tag{2-29}$$

Indeed, consider, for example, $Q_2\widehat{T}(\lambda)A(\lambda)\widehat{T}(\lambda)Q_2$. It can be reexpressed as

$$Q_2\widehat{T}(\lambda)A(\lambda)\widehat{T}(\lambda)Q_2 = \lambda^4 Q_2 V_2 \frac{R_0((\lambda+i0)^2)-R_0(0)-i\lambda\frac{1\otimes 1}{4\pi}}{\lambda^2} V_1 A(\lambda) V_2 \frac{R_0((\lambda+i0)^2)-R_0(0)-i\lambda\frac{1\otimes 1}{4\pi}}{\lambda^2} V_1 Q_2. \tag{2-30}$$

For this computation, we assume that $V \in \langle x\rangle^{-4} L^{\frac{3}{2},1}$. Taking a derivative of (2-30), we obtain terms such as

$$Q_2 V_2 \partial_\lambda\left(\frac{R_0((\lambda+i0)^2)-R_0(0)-i\lambda\frac{1\otimes 1}{4\pi}}{\lambda^2}\right) V_1 A(\lambda) V_2 \frac{R_0((\lambda+i0)^2)-R_0(0)-i\lambda\frac{1\otimes 1}{4\pi}}{\lambda^2} V_1 Q_2. \tag{2-31}$$

Note that the range of Q_2 is spanned by functions $V_2\phi_k$, with $2 \le k \le N$, such that $|\phi_k(y)| \lesssim \langle y\rangle^{-2}$ and $V_2 \in \langle x\rangle^{-2} L^{3,2}$, so $V_2\phi \in \langle y\rangle^{-4} L^{3,2}$. Also

$$M\left(\left(V_2\partial_\lambda\left(\frac{R_0((\lambda+i0)^2)-R_0(0)-i\lambda\frac{1\otimes 1}{4\pi}}{\lambda^2}\right)V_1\right)^{\wedge}\right) = |V_2|\frac{|x-y|^2}{24\pi}|V_1| \in \mathcal{B}(L^{\frac{3}{2},2}, L^{3,2}).$$

Likewise

$$M\left(\left(V_2\frac{R_0((\lambda+i0)^2)-R_0(0)-i\lambda\frac{1\otimes 1}{4\pi}}{\lambda^2}V_1\right)^{\wedge}\right) = |V_2|\frac{|x-y|}{8\pi}|V_1| \in \mathcal{B}(L^{\frac{3}{2},2}, L^{\frac{3}{2},2}).$$

This shows that (2-31) $\in \mathcal{V}_{L^{3/2,2},L^{3,2}}$. By such computations, we obtain that $Q_2\widehat{T}(\lambda)A(\lambda)\widehat{T}(\lambda)Q_2 = \lambda^4 E_{22}(\lambda)$, where $\chi\big(\frac{\lambda}{\epsilon}\big)E_{22}(\lambda) \in \mathcal{W}$ for sufficiently small ϵ. In this manner, we prove (2-29).

By (2-26), we have $S_{11}^{-1}(\lambda) = (Q\widehat{T}(\lambda)Q)^{-1}$ is of the form

$$S_{11}^{-1}(\lambda) = \begin{pmatrix} \lambda^{-1}E(\lambda) & \lambda^{-1}E(\lambda) \\ \lambda^{-1}E(\lambda) & \lambda^{-2}E(\lambda) \end{pmatrix}.$$

Then, letting $N(\lambda) := S_{11}^{-1}(\lambda)S_{10}(\lambda)A(\lambda)S_{01}(\lambda)$, by (2-29),

$$\begin{aligned} N(\lambda) &:= S_{11}^{-1}(\lambda)S_{10}(\lambda)S_{00}^{-1}(\lambda)S_{01}(\lambda) \\ &= \begin{pmatrix} \lambda^{-1}E(\lambda) & \lambda^{-1}E(\lambda) \\ \lambda^{-1}E(\lambda) & \lambda^{-2}E(\lambda) \end{pmatrix} \begin{pmatrix} \lambda^2 E_{11}(\lambda) & \lambda^3 E_{12}(\lambda) \\ \lambda^3 E_{21}(\lambda) & \lambda^4 E_{22}(\lambda) \end{pmatrix} \\ &= \begin{pmatrix} \lambda E(\lambda) & \lambda^2 E(\lambda) \\ \lambda E(\lambda) & \lambda^2 E(\lambda) \end{pmatrix}. \end{aligned}$$

This shows that $C(\lambda)$ is invertible for $\lambda \ll 1$:

$$C(\lambda) = S_{11}(\lambda) - S_{10}(\lambda)A(\lambda)S_{01}(\lambda) = S_{11}(\lambda)(1 - N(\lambda)),$$

so

$$\begin{aligned} C^{-1}(\lambda) &= (I - N(\lambda))^{-1} S_{11}^{-1}(\lambda) \\ &= S_{11}^{-1}(\lambda) + (I - N(\lambda))^{-1} N(\lambda) S_{11}^{-1}(\lambda). \end{aligned} \tag{2-32}$$

A computation shows that $(I-N(\lambda))^{-1}N(\lambda)S_{11}^{-1}(\lambda)$ is a regular term:

$$(1-N(\lambda))^{-1}N(\lambda)S_{11}^{-1}(\lambda) = E(\lambda)\begin{pmatrix}\lambda E(\lambda) & \lambda^2 E(\lambda)\\ \lambda E(\lambda) & \lambda^2 E(\lambda)\end{pmatrix}\begin{pmatrix}\lambda^{-1}E(\lambda) & \lambda^{-1}E(\lambda)\\ \lambda^{-1}E(\lambda) & \lambda^{-2}E(\lambda)\end{pmatrix} = E(\lambda).$$

By (2-32) and (2-27),

$$\begin{aligned}C^{-1}(\lambda) &= S_{11}^{-1}(\lambda)+E(\lambda)\\ &= \lambda^{-2}V_2P_0V_1 + i\lambda^{-1}V_2P_0V\frac{|x-y|^2}{24}VP_0V_1 - a\lambda^{-1}V_2\phi\otimes V_1\phi + E(\lambda).\end{aligned}$$

One can then also write C^{-1} as

$$C^{-1}(\lambda) = \begin{pmatrix}\lambda^{-1}E(\lambda) & \lambda^{-1}E(\lambda)\\ \lambda^{-1}E(\lambda) & \lambda^{-2}E(\lambda)\end{pmatrix}.$$

We also have

$$S_{01}(\lambda) = \overline{Q}(I+\widehat{T}(\lambda))Q = \lambda E_1(\lambda)Q_1 + \lambda^2 E_2(\lambda)Q_2$$

with regular terms $E_1, E_2 \in \mathcal{W}$:

$$\begin{aligned}E_1(\lambda) &:= \overline{Q}V_2\frac{R_0((\lambda+i0)^2)-R_0(0)}{\lambda}V_1Q_1,\\ E_2(\lambda) &:= \overline{Q}V_2\frac{R_0((\lambda+i0)^2)-R_0(0)-i\lambda 1\otimes 1}{\lambda^2}V_1Q_2.\end{aligned}$$

Showing that $E_1, E_2 \in \mathcal{W}$ requires assuming that $V \in \langle x\rangle^{-4}L^{\frac{3}{2},1}$.

Therefore, the following matrix element of (2-28) is regular near zero:

$$A(\lambda)S_{01}(\lambda)C^{-1}(\lambda) = \big(\lambda A(\lambda)E_1(\lambda)\ \lambda^2 A(\lambda)E_2(\lambda)\big)\begin{pmatrix}\lambda^{-1}E(\lambda) & \lambda^{-1}E(\lambda)\\ \lambda^{-1}E(\lambda) & \lambda^{-2}E(\lambda)\end{pmatrix} = E(\lambda).$$

One shows in the same manner that the matrix element $C^{-1}(\lambda)S_{10}(\lambda)A(\lambda)$ of (2-28) is regular near zero.

Finally, the last remaining matrix element $A + AS_{01}C^{-1}S_{10}A$ of (2-28) consists of the regular part A and

$$\begin{aligned}AS_{01}C^{-1}S_{10}A &= E(\lambda)\big(\lambda E(\lambda)\ \ \lambda^2 E(\lambda)\big)\begin{pmatrix}\lambda^{-1}E(\lambda) & \lambda^{-1}E(\lambda)\\ \lambda^{-1}E(\lambda) & \lambda^{-2}E(\lambda)\end{pmatrix}\begin{pmatrix}\lambda E(\lambda)\\ \lambda^2 E(\lambda)\end{pmatrix}E(\lambda)\\ &= \lambda E(\lambda).\end{aligned}$$

Thus this is also a regular term. It follows by (2-28) that $\widehat{T}(\lambda)^{-1}$ is up to regular terms given by

$$\lambda^{-2}V_2P_0V_1 + i\lambda^{-1}V_2P_0V\frac{|x-y|^2}{24}VP_0V_1 - a\lambda^{-1}V_2\phi\otimes V_1\phi,$$

which was to be shown. □

We next prove a corresponding statement in the case when V has an almost minimal amount of decay. One can also obtain a resolvent expansion when $V \in \langle x\rangle^{-1}L^{\frac{3}{2},1}$, but it does not lead to decay estimates.

Lemma 2.17. *Suppose that $V \in \langle x\rangle^{-2} L^{\frac{3}{2},1}$ and $H = -\Delta + V$ is an exceptional Hamiltonian of the third kind. Let χ be a standard cutoff function. Then, for sufficiently small ϵ,*

$$\chi\Big(\frac{\lambda}{\epsilon}\Big)(I+\widehat{T}(\lambda))^{-1} = L(\lambda) + \lambda^{-1} S(\lambda) + \lambda^{-2} V_2 P_0 V_1,$$

where $L(\lambda) \in \mathcal{W}$, $S(\lambda)^\vee \in \mathcal{V}_{L^{3,2}, L^{3/2,2}}$, and P_0 is the L^2 orthogonal projection on $\mathcal{E}$.

Furthermore, 0 is an isolated exceptional point, so H has finitely many negative eigenvalues.

Proof of Lemma 2.17. We study $(I+\widehat{T}(\lambda))^{-1} := \big(I + V_2 R_0((\lambda+i0)^2) V_1\big)^{-1}$ near $\lambda = 0$.

Let $Q = Q_1 + Q_2$, $Q_0 = \overline{Q}$, and Q_1 and Q_2 be as in the proof of Lemma 2.16.

Also take again the orthonormal basis $\{\phi_1, \dots, \phi_N\}$ with respect to the inner product $-(Vu, v)$ for $\mathcal{M}$ so that $\{\phi_2, \dots, \phi_N\}$ is a basis of $\mathcal{E}$ and $\langle \phi_1, V\rangle > 0$.

We apply Lemma 2.10 to invert $Q(I+\widehat{T}(\lambda))Q$ in QL^2 for small λ, after writing it in matrix form with respect to the decomposition $QL^2 = Q_1 L^2 + Q_2 L^2$:

$$Q(I+\widehat{T}(\lambda))Q = \begin{pmatrix} Q_1(I+\widehat{T}(\lambda))Q_1 & Q_1\widehat{T}(\lambda)Q_2 \\ Q_2\widehat{T}(\lambda)Q_1 & Q_2(I+\widehat{T}(\lambda))Q_2 \end{pmatrix} := \begin{pmatrix} T_{11}(\lambda) & T_{12}(\lambda) \\ T_{21}(\lambda) & T_{22}(\lambda) \end{pmatrix}.$$

The inverse will be given by formula (2-13), that is,

$$(Q(I+\widehat{T}(\lambda))Q)^{-1} = \begin{pmatrix} T_{11}^{-1} + T_{11}^{-1} T_{12} C_{22}^{-1} T_{21} T_{11}^{-1} & -T_{11}^{-1} T_{12} C_{22}^{-1} \\ -C_{22}^{-1} T_{21} T_{11}^{-1} & C_{22}^{-1} \end{pmatrix}, \tag{2-33}$$

where

$$C_{22} = T_{22} - T_{21} T_{11}^{-1} T_{12}.$$

Then (recall that $Q_1 = -V_2\phi_1 \otimes V_1\phi_1$),

$$\begin{aligned} T_{11}(\lambda) &= Q_1(I+\widehat{T}(\lambda))Q_1 = Q_1\big(I + V_2 R_0((\lambda+i0)^2)V_1\big)Q_1 \\ &= Q_1\big(V_2 R_0((\lambda+i0)^2)V_1 - V_2 R_0(0) V_1\big)Q_1 \\ &= V_2\phi_1 \otimes V\phi_1 \big(R_0((\lambda+i0)^2) - R_0(0)\big) V\phi_1 \otimes V_1\phi_1 \\ &=: \lambda c_0(\lambda) Q_1. \end{aligned}$$

Here $c_0(0) = a = 4i\pi/|\langle V, \phi_1\rangle|^2 \neq 0$. Note that $c_0(\lambda) \in \widehat{L}^1$ when

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} V(x)\phi_1(x) V(y)\phi_1(y) \bigg\| \frac{e^{i\lambda|x-y|} - 1}{\lambda|x-y|} \bigg\|_{\widehat{L}^1_\lambda} dx\, dy < \infty.$$

Since

$$\bigg\| \frac{e^{i\lambda|x-y|} - 1}{\lambda|x-y|} \bigg\|_{\widehat{L}^1_\lambda} = 1,$$

it is enough to assume that $V\phi_1 \in L^1$, i.e., that $V \in L^{\frac{3}{2},1}$, in view of the fact that $\phi_1 \in \langle x\rangle^{-1} L^\infty$.

It follows that $T_{11}(\lambda)$ is invertible for $|\lambda| \ll 1$ in $Q_1 L^2$ and

$$T_{11}^{-1}(\lambda) = \lambda^{-1} c_0^{-1}(\lambda) Q_1 = \lambda^{-1} E(\lambda).$$

Here $\chi\big(\frac{\lambda}{\epsilon}\big)c_0^{-1}(\lambda) \in \widehat{L}^1$ for sufficiently small ϵ.

Likewise, since $Q_2(V_2 \otimes V_1) = (V_2 \otimes V_1)Q_2 = 0$,

$$\begin{aligned} T_{12}(\lambda) &= Q_1\big(I + V_2 R_0((\lambda+i0)^2)V_1\big)Q_2 \\ &= \lambda^2 Q_1 V_2 \frac{R_0((\lambda+i0)^2) - R_0(0) - i\lambda(4\pi)^{-1} 1 \otimes 1}{\lambda^2} V_1 Q_2 \\ &= \lambda^2 Q_1 e(\lambda) Q_2. \end{aligned}$$

Since by Lemma 2.6

$$M\bigg(\bigg(\frac{R_0((\lambda+i0)^2) - R_0(0) - i\lambda(4\pi)^{-1} 1 \otimes 1}{\lambda^2}\bigg)^{\wedge}\bigg) = \frac{|x-y|}{8\pi},$$

it follows that $e(\lambda) \in \widehat{L}^1$ if

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} V(x)\phi_1(x)V(y)\phi_k(y)|x-y| < \infty,$$

that is, if $V \in L^1$.

Likewise we obtain $T_{21}(\lambda) = \lambda^2 Q_2 e(\lambda) Q_1$; hence, combining the previous results,

$$T_{21}(\lambda)T_{11}^{-1}(\lambda)T_{12}(\lambda) = \lambda^3 Q_2 e(\lambda) Q_2.$$

Furthermore,

$$\begin{aligned} T_{22}(\lambda) &= Q_2\big(I + V_2 R_0((\lambda+i0)^2)V_1\big)Q_2 \\ &= \lambda^2 Q_2 V_2 \frac{R_0((\lambda+i0)^2) - R_0(0) - i\lambda\frac{1\otimes 1}{4\pi}}{\lambda^2} V_1 Q_2 \\ &= -\lambda^2\bigg(Q_2 V_2 \frac{|x-y|}{8\pi} V_1 Q_2 + \lambda Q_2 e(\lambda) Q_2\bigg). \end{aligned}$$

Again by Lemma 2.6, $e(\lambda) \in \widehat{L}^1$ if

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} V(x)\phi_k(x)V(y)\phi_\ell(y)|x-y|^2 < \infty,$$

that is (taking into account that $\phi_k, \phi_\ell \lesssim \langle x\rangle^{-2}$), if $V \in L^1$.

Let P_0 be the L^2 orthogonal projection onto the set $\mathcal{E}$ spanned by $\phi_2, \dots, \phi_N$. By relation (4.38) of [Yajima 2005],

$$\Big(Q_2 V_2 \frac{|x-y|}{8\pi} V_1 Q_2\Big)^{-1} = -V_2 P_0 V_1.$$

Then

$$\begin{aligned} C_{22}(\lambda) &= T_{22}(\lambda) - T_{21}(\lambda)T_{11}^{-1}(\lambda)T_{12}(\lambda) \\ &= -\lambda^2 Q_2 V_2 \frac{|x-y|}{8\pi} V_1 Q_2 + \lambda^3 Q_2 e(\lambda) Q_2. \end{aligned}$$

Therefore,

$$C_{22}^{-1}(\lambda) = \lambda^{-2} V_2 P_0 V_1 + \lambda^{-1} Q_2 e(\lambda) Q_2.$$

Furthermore, we then obtain that

$$\begin{aligned} -T_{11}^{-1}(\lambda)T_{12}(\lambda)C_{22}^{-1}(\lambda) &= \lambda^{-1}Q_1e(\lambda)Q_1\lambda^2Q_1e(\lambda)Q_2\lambda^{-2}Q_2e(\lambda)Q_2 \\ &= \lambda^{-1}Q_1e(\lambda)Q_2. \end{aligned}$$

Likewise we obtain

$$\begin{aligned} -C_{22}^{-1}(\lambda)T_{21}(\lambda)T_{11}^{-1}(\lambda) &= \lambda^{-1}Q_2e(\lambda)Q_1, \\ T_{11}^{-1}(\lambda)T_{12}(\lambda)C_{22}^{-1}(\lambda)T_{21}(\lambda)T_{11}^{-1}(\lambda) &= Q_1e(\lambda)Q_1. \end{aligned}$$

By (2-33), we know that $\big(Q(I+\widehat{T}(\lambda))Q\big)^{-1}$ is given in matrix form by

$$\big(Q(I+\widehat{T}(\lambda))Q\big)^{-1} = \begin{pmatrix} \lambda^{-1}Q_1e(\lambda)Q_1 & \lambda^{-1}Q_1e(\lambda)Q_2 \\ \lambda^{-1}Q_2e(\lambda)Q_1 & \lambda^{-2}V_2P_0V_1+\lambda^{-1}Q_2e(\lambda)Q_2 \\ & \lambda^{-1}Qe(\lambda)Q+\lambda^{-2}V_2P_0V_1 \end{pmatrix}, \tag{2-34}$$

where $\chi\big(\frac{\lambda}{\epsilon}\big)e(\lambda)\in\widehat{L}^1$ for sufficiently small ϵ.

We apply Lemma 2.10 again after writing $I+\widehat{T}(\lambda)$ in matrix form with respect to the decomposition $L^2=\overline{Q}L^2+QL^2$, where $QL^2=V_2\mathcal{M}$:

$$I+\widehat{T}(\lambda) = \begin{pmatrix} \overline{Q}(I+\widehat{T}(\lambda))\overline{Q} & \overline{Q}\widehat{T}(\lambda)Q \\ Q\widehat{T}(\lambda)\overline{Q} & Q(I+\widehat{T}(\lambda))Q \end{pmatrix} := \begin{pmatrix} S_{00}(\lambda) & S_{01}(\lambda) \\ S_{10}(\lambda) & S_{11}(\lambda) \end{pmatrix}.$$

Next, as in the proof of Lemma 2.16, let $A(\lambda)=S_{00}^{-1}(\lambda)$. Then $\chi\big(\frac{\lambda}{\epsilon}\big)A(\lambda)\in\mathcal{W}$ for sufficiently small ϵ.

We compute the inverse of $I+\widehat{T}(\lambda)$ by finding each of its matrix elements:

$$(I+\widehat{T}(\lambda))^{-1} = \begin{pmatrix} A+AS_{01}C^{-1}S_{10}A & AS_{01}C^{-1} \\ -C^{-1}S_{10}A & C^{-1} \end{pmatrix}. \tag{2-35}$$

Here

$$C(\lambda)=S_{11}(\lambda)-S_{10}(\lambda)A(\lambda)S_{01}(\lambda).$$

$S_{10}(\lambda)A(\lambda)S_{01}(\lambda)=Q\widehat{T}(\lambda)A(\lambda)\widehat{T}(\lambda)Q$ may be written as

$$\begin{pmatrix} Q_1\widehat{T}(\lambda)A(\lambda)\widehat{T}(\lambda)Q_1 & Q_1\widehat{T}(\lambda)A(\lambda)\widehat{T}(\lambda)Q_2 \\ Q_2\widehat{T}(\lambda)A(\lambda)\widehat{T}(\lambda)Q_1 & Q_2\widehat{T}(\lambda)A(\lambda)\widehat{T}(\lambda)Q_2 \end{pmatrix} = \begin{pmatrix} \lambda^2Q_1e(\lambda)Q_1 & \lambda^3Q_1e(\lambda)Q_2 \\ \lambda^3Q_2e(\lambda)Q_1 & \lambda^3Q_2e(\lambda)Q_2 \end{pmatrix}, \tag{2-36}$$

where $e(\lambda)\in\widehat{L}^1$.

Indeed, consider, for example, $Q_2\widehat{T}(\lambda)A(\lambda)\widehat{T}(\lambda)Q_2$. It can be rewritten as

$$\begin{aligned} &Q_2\widehat{T}(\lambda)A(\lambda)\widehat{T}(\lambda)Q_2 \\ &\quad=\lambda^3Q_2V_2\frac{R_0((\lambda+i0)^2)-R_0(0)-i\lambda 1\otimes 1}{\lambda}V_1A(\lambda)V_2\frac{R_0((\lambda+i0)^2)-R_0(0)}{\lambda}V_1Q_2. \end{aligned} \tag{2-37}$$

Assuming that $V\in\langle x\rangle^{-2}L^{\frac{3}{2},1}$,

$$M\bigg(\Big(V_2\frac{R_0((\lambda+i0)^2)-R_0(0)}{\lambda}V_1\Big)^{\wedge}\bigg) = \frac{|V_2|\otimes|V_1|}{4\pi}\in\mathcal{B}(L^{\frac{3}{2},2}).$$

Likewise

$$M\left(\left(V_2\frac{R_0((\lambda+i0)^2)-R_0(0)-i\lambda\frac{1\otimes 1}{4\pi}}{\lambda^2}V_1\right)^{\wedge}\right)=|V_2|\frac{|x-y|}{8\pi}|V_1|\in\mathcal{B}(L^{\frac{3}{2},2},L^{3,2}).$$

This implies that (2-37) $=\lambda^3Q_2e_0(\lambda)Q_2$ and $e_0(\lambda)\in\widehat{L}^1$. In this manner, we prove (2-36).

By (2-34), we know that $S_{11}^{-1}(\lambda)=(Q\widehat{T}(\lambda)Q)^{-1}$ is of the form

$$S_{11}^{-1}(\lambda)=\begin{pmatrix}\lambda^{-1}Q_1e(\lambda)Q_1 & \lambda^{-1}Q_1e(\lambda)Q_2\\ \lambda^{-1}Q_2e(\lambda)Q_1 & \lambda^{-2}Q_2e(\lambda)Q_2\end{pmatrix}.$$

Then, letting $N(\lambda):=S_{11}^{-1}(\lambda)S_{10}(\lambda)A(\lambda)S_{01}(\lambda)$, by (2-36),

$$\begin{aligned}N(\lambda)&:=S_{11}^{-1}(\lambda)S_{10}(\lambda)S_{00}^{-1}(\lambda)S_{01}(\lambda)\\&=\begin{pmatrix}\lambda^{-1}Q_1e(\lambda)Q_1 & \lambda^{-1}Q_1e(\lambda)Q_2\\ \lambda^{-1}Q_2e(\lambda)Q_1 & \lambda^{-2}Q_2e(\lambda)Q_2\end{pmatrix}\begin{pmatrix}\lambda^{2}Q_1e(\lambda)Q_1 & \lambda^{3}Q_1e(\lambda)Q_2\\ \lambda^{3}Q_2e(\lambda)Q_1 & \lambda^{3}Q_2e(\lambda)Q_2\end{pmatrix}\\&=\begin{pmatrix}\lambda Q_1e(\lambda)Q_1 & \lambda^{2}Q_1e(\lambda)Q_2\\ \lambda Q_2e(\lambda)Q_1 & \lambda Q_2e(\lambda)Q_2\end{pmatrix}.\end{aligned}$$

Therefore $N(0)=0$. This shows that $C(\lambda)$ is invertible for $\lambda\ll 1$:

$$C(\lambda)=S_{11}(\lambda)-S_{10}(\lambda)A(\lambda)S_{01}(\lambda)=S_{11}(\lambda)(I-N(\lambda)),$$

so

$$\begin{aligned}C^{-1}(\lambda)&=(I-N(\lambda))^{-1}S_{11}^{-1}(\lambda)\\&=S_{11}^{-1}(\lambda)+(I-N(\lambda))^{-1}N(\lambda)S_{11}^{-1}(\lambda).\end{aligned}\tag{2-38}$$

A computation shows that

$$\begin{aligned}(I-N(\lambda))^{-1}N(\lambda)S_{11}^{-1}(\lambda)&=Qe(\lambda)Q\begin{pmatrix}\lambda Q_1e(\lambda)Q_1 & \lambda^{2}Q_1e(\lambda)Q_2\\ \lambda Q_2e(\lambda)Q_1 & \lambda Q_2e(\lambda)Q_2\end{pmatrix}\begin{pmatrix}\lambda^{-1}Q_1e(\lambda)Q_1 & \lambda^{-1}Q_1e(\lambda)Q_2\\ \lambda^{-1}Q_2e(\lambda)Q_1 & \lambda^{-2}Q_2e(\lambda)Q_2\end{pmatrix}\\&=\begin{pmatrix}Q_1e(\lambda)Q_1 & Q_1e(\lambda)Q_2\\ Q_2e(\lambda)Q_1 & \lambda^{-1}Q_2e(\lambda)Q_2\end{pmatrix}.\end{aligned}$$

By (2-38) and (2-34),

$$\begin{aligned}C^{-1}(\lambda)&=S_{11}^{-1}(\lambda)+\lambda^{-1}Qe(\lambda)Q\\&=\lambda^{-2}V_2P_0V_1+\lambda^{-1}Qe(\lambda)Q.\end{aligned}$$

Note that

$$\begin{aligned}S_{01}(\lambda)&=\overline{Q}\widehat{T}(\lambda)Q=\overline{Q}(I+\widehat{T}(\lambda))Q\\&=\lambda\overline{Q}V_2\frac{R_0((\lambda+i0)^2)-R_0(0)}{\lambda}V_1Q=\lambda E_1(\lambda),\end{aligned}$$

where $E_1(\lambda)^{\vee}\in\mathcal{V}_{L^{3/2,2}}$ when $V\in\langle x\rangle^{-1}L^1$. Therefore,

$$A(\lambda)S_{01}(\lambda)C^{-1}(\lambda)=A(\lambda)\lambda E_1(\lambda)\lambda^{-2}Qe(\lambda)Q=\lambda^{-1}S(\lambda),$$

where $S(\lambda)^\vee \in \mathcal{V}_{L^{3,2},L^{3/2,2}}$. Likewise $S_{10}(\lambda)=\lambda E_2(\lambda)$, where $E_2(\lambda)^\vee \in \mathcal{V}_{L^{3,2}}$. Then

$$C^{-1}(\lambda)S_{10}(\lambda)A(\lambda)=\lambda^{-1}S(\lambda),$$

where $S(\lambda)^\vee \in \mathcal{V}_{L^{3,2},L^{3/2,2}}$.

Finally, for the last remaining matrix element $A+AS_{01}C^{-1}S_{10}A$ of (2-35), we use the fact that

$$AS_{01}C^{-1}S_{10}A=A(\lambda)\lambda E_1(\lambda)\lambda^{-2}Qe(\lambda)Q\lambda E_2(\lambda)A(\lambda)=S(\lambda),$$

where $S(\lambda)^\vee \in \mathcal{V}_{L^{3,2},L^{3/2,2}}$. Also recall that $A(\lambda)\in\mathcal{W}$.

We have thus analyzed all the terms in (2-35) and the conclusion follows. □

Recall that

$$R(t):=\frac{ae^{-i\frac{3\pi}{4}}}{\sqrt{\pi t}}\zeta_t(x)\otimes\zeta_t(y),\ \zeta_t(x):=e^{i\frac{|x|^2}{4t}}\phi(x),$$

$$S(t):=\frac{e^{-i\frac{3\pi}{4}}}{\sqrt{\pi t}}\Big(-iP_0V\frac{|x-y|^2}{24\pi}VP_0+\mu_t(x)\frac{|x-y|}{8\pi}VP_0+P_0V\frac{|x-y|}{8\pi}\mu_t(y)\Big),$$

where

$$\mu_t(x):=\frac{i}{|x|}\int_0^1(e^{i\frac{|x|^2}{4t}}-e^{i\frac{|\theta x|^2}{4t}})\,d\theta.$$

Although it is not immediately obvious, it is also true that

$$\|S(t)u\|_{L^{3,\infty}}\lesssim t^{-\frac{1}{2}}\|u\|_{L^{3/2,1}}. \tag{2-39}$$

Indeed, note that since $\langle\phi_k,V\rangle=0$ for the eigenvectors ϕ_k, with $2\le k\le N$ (recall that ϕ_1 is the resonance),

$$\mu_t(x)|x-y|VP_0=\mu_t(x)(|x-y|-|x|)VP_0,$$

which is bounded in absolute value by

$$\sum_{k=2}^{N}|\mu_t(x)|\int_{\mathbb{R}^3}|y||V(y)||\phi_k(y)|\,dy\otimes|\phi_k(z)|.$$

By definition, $|\mu_t(x)|\lesssim|x|^{-1}$. This leads to (2-39), since $\phi_k\in\langle x\rangle^{-2}L^\infty$ and $V\in L^{\frac{3}{2},1}$.

We use Lemma 2.16 as the basis for the following decay estimate:

Proposition 2.18. *Let V satisfy $\langle x\rangle^4V(x)\in L^{\frac{3}{2},1}$. Suppose that H is of exceptional type of the third kind. Then, for $1\le p<\frac{3}{2}$ and $u\in L^2\cap L^p$,*

$$e^{-itH}P_cu=Z(t)u+R(t)u+S(t)u,\quad \|Z(t)u\|_{L^{p'}}\lesssim t^{-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{p'}\right)}\|u\|_{L^p}. \tag{2-40}$$

Here $\frac{1}{p}+\frac{1}{p'}=1$. If in addition all the zero-energy eigenfunctions ϕ_k, with $2\le k\le N$, are in L^1, then we can take $S(t)=0$.

Proof of Proposition 2.18. Write the dispersive component of the evolution as

$$e^{itH} P_c f = \frac{1}{i\pi} \int_{\mathbb{R}} e^{it\lambda^2} \big(R_0((\lambda+i0)^2) - R_0((\lambda+i0)^2) V_1 \hat{T}(\lambda)^{-1} V_2 R_0((\lambda+i0)^2)\big) f \, \lambda \, d\lambda.$$

We use the same method as in the proofs of Propositions 2.13 and 2.15. Consider a partition of unity subordinated to the neighborhoods of Lemmas 2.8 and 2.16. First, following Lemma 2.8, take a sufficiently large R such that

$$\Big(1-\chi\Big(\frac{\lambda}{R}\Big)\Big)(I+\hat{T}(\lambda))^{-1} \in \mathcal{W}.$$

Then, again by Lemma 2.8, for every $\lambda_0 \in [-4R, 4R]$, there exists $\epsilon(\lambda_0) > 0$ such that

$$\chi\Big(\frac{\lambda-\lambda_0}{\epsilon(\lambda_0)}\Big)(I+\hat{T}(\lambda))^{-1} \in \mathcal{W}$$

if $\lambda_0 \neq 0$ while the conclusion of Lemma 2.16 holds when $\lambda_0 = 0$.

Since $[-4R, 4R]$ is a compact set, there exists a finite covering

$$[-4R, 4R] \subset \bigcup_{k=1}^{N} \big(\lambda_k - \epsilon(\lambda_k), \lambda_k + \epsilon(\lambda_k)\big).$$

Then we construct a finite partition of unity on $\mathbb{R}$ by smooth functions $1 = \chi_0(\lambda) + \sum_{k=1}^{N} \chi_k(\lambda) + \chi_\infty(\lambda)$, where $\operatorname{supp} \chi_\infty \subset \mathbb{R} \setminus (-2R, 2R)$, $\operatorname{supp} \chi_0 \subset [-\epsilon(0), \epsilon(0)]$, and $\operatorname{supp} \chi_k \subset \big[\lambda_k - \epsilon(\lambda_k), \lambda_k + \epsilon(\lambda_k)\big]$.

By Lemma 2.8, for any $k \neq 0$, we have $\chi_k(\lambda)(I+\hat{T}(\lambda))^{-1} \in \mathcal{W}$, so $(1-\chi_0(\lambda))(I+\hat{T}(\lambda))^{-1} \in \mathcal{W}$. By Lemma 2.16, for $L \in \mathcal{W}$,

$$\chi_0(\lambda)(I+\hat{T}(\lambda))^{-1} = L(\lambda) + \chi_0(\lambda)\Big(\frac{V_2 P_0 V_1}{\lambda^2} + \frac{i V_2 P_0 V |x-y|^2 V P_0 V_1}{\lambda} - \frac{a}{\lambda} V_2 \phi \otimes V_1 \phi\Big).$$

Let Z_1 be the contribution of all the regular terms in this decomposition, such as the free resolvent, $(1-\chi_0(\lambda))(I+\hat{T}(\lambda))^{-1}$, and $L(\lambda)$:

$$\begin{aligned} Z_1(t) &:= \frac{1}{i\pi} \int_{\mathbb{R}} e^{-it\lambda^2} \big(R_0((\lambda+i0)^2) - R_0((\lambda+i0)^2) V_1 L(\lambda) V_2 R_0((\lambda+i0)^2) \\ &\qquad - (1-\chi_0(\lambda)) R_0((\lambda+i0)^2) V_1 \hat{T}(\lambda) V_2 R_0((\lambda+i0)^2)\big) \lambda \, d\lambda \\ &= \frac{1}{2\pi t} \int_{\mathbb{R}} e^{-it\lambda^2} \partial_\lambda \big(R_0((\lambda+i0)^2) - R_0((\lambda+i0)^2) V_1 L(\lambda) V_2 R_0((\lambda+i0)^2) \\ &\qquad - (1-\chi_0(\lambda)) R_0((\lambda+i0)^2) V_1 \hat{T}(\lambda) V_2 R_0((\lambda+i0)^2)\big) \, d\lambda \\ &= \frac{C}{t^{\frac{3}{2}}} \int_{\mathbb{R}} e^{-i\frac{\rho^2}{4t}} \big(\partial_\lambda \big(R_0((\lambda+i0)^2) - R_0((\lambda+i0)^2) V_1 L(\lambda) V_2 R_0((\lambda+i0)^2) \\ &\qquad - (1-\chi_0(\lambda)) R_0((\lambda+i0)^2) V_1 \hat{T}(\lambda) V_2 R_0((\lambda+i0)^2)\big)\big)^\vee(\rho) \, d\rho. \end{aligned}$$

The fact that $\|Z_1(t)u\|_{L^1} \lesssim |t|^{-\frac{3}{2}} \|u\|_{L^\infty}$ follows by knowing that

$$\begin{aligned} &\big(\partial_\lambda \big(R_0((\lambda+i0)^2) - R_0((\lambda+i0)^2) V_1 L(\lambda) V_2 R_0((\lambda+i0)^2) \\ &\qquad - (1-\chi_0(\lambda)) R_0((\lambda+i0)^2) V_1 \hat{T}(\lambda) V_2 R_0((\lambda+i0)^2)\big)\big)^\vee \in \mathcal{V}_{L^1, L^\infty}. \end{aligned}$$

By smoothing estimates, it also follows that $Z_1(t)$ is L^2-bounded; see the proof of Proposition 2.13. By interpolation, we also obtain the estimate $\|Z_1(t)u\|_{L^{3,\infty}} \lesssim \|u\|_{L^{3/2,1}}$.

Let $Z_2(t)$ be the contribution of the term $a\lambda^{-1}\chi_0(\lambda)V_2\phi \otimes V_1\phi$:

$$Z_2(t) := \frac{a}{i\pi}\int_{\mathbb{R}} e^{-it\lambda^2}\chi_0(\lambda)R_0((\lambda+i0)^2)V\phi \otimes V\phi R_0((\lambda+i0)^2)\,d\lambda.$$

By Lemma 2.14,

$$\|(Z_2(t)-R(t))u\|_{L^\infty} \le t^{-\frac{3}{2}}\|u\|_{L^1}, \quad \|Z_2(t)u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}}\|u\|_{L^{3/2,1}}.$$

We are left with the terms

$$\lambda^{-2}R_0((\lambda+i0)^2)VP_0VR_0((\lambda+i0)^2) \quad \text{and} \quad i\lambda^{-1}R_0((\lambda+i0)^2)VP_0V\frac{|x-y|^2}{24\pi}VP_0VR_0((\lambda+i0)^2).$$

Let their contributions be

$$X_2(t) := \frac{-1}{\pi}\int_{\mathbb{R}} e^{-it\lambda^2}R_0((\lambda+i0)^2)VP_0V\frac{|x-y|^2}{24\pi}VP_0VR_0((\lambda+i0)^2)\,d\lambda,$$
$$X_3(t) := \frac{-1}{i\pi}\lim_{\delta\to 0}\int_{|\lambda|>\delta} e^{-it\lambda^2}R_0((\lambda+i0)^2)VP_0VR_0((\lambda+i0)^2)\lambda^{-1}\,d\lambda.$$

By [Yajima 2005, Lemma 4.12],

$$\begin{aligned}&\|X_2(t)u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}}\|u\|_{L^{3/2,1}},\\ &\left\|X_2(t)u + i\frac{e^{-i\frac{3\pi}{4}}}{\sqrt{\pi t}}P_0V\frac{|x-y|^2}{24\pi}VP_0\right\|_{L^\infty} \lesssim t^{-\frac{3}{2}}\|u\|_{L^1}.\end{aligned} \tag{2-41}$$

This lemma has a proof similar to Lemma 2.14. It requires, in addition, that $|\phi_j(x)| \lesssim |x|^{-2}$ for every eigenfunction $\phi_j \in \mathcal{E}$, with $2 \le j \le N$, which is guaranteed by Lemma 2.3.

By [Yajima 2005, Lemma 4.14],

$$\begin{aligned}&\|X_3(t)u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}}\|u\|_{L^{3/2,1}},\\ &\left\|X_3(t)u - \frac{e^{-i\frac{3\pi}{4}}}{\sqrt{\pi t}}\left(\mu_t(x)\frac{|x-y|}{8\pi}VP_0 + P_0V\frac{|x-y|}{8\pi}\mu_t(y)\right)\right\|_{L^\infty} \lesssim t^{-\frac{3}{2}}\|u\|_{L^1}.\end{aligned} \tag{2-42}$$

The proof of [Yajima 2005, Lemma 4.14] depends on $\langle y\rangle^3 V(y)\phi(y)$ being integrable, which is also true here since $|\phi(y)| \lesssim \langle y\rangle^{-1}$ and $\langle y\rangle^2 V(y) \in \langle y\rangle^{-2}L^{\frac{3}{2},1} \subset L^1$.

Combining the two results (2-41) and (2-42) and knowing that $\|S(t)u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}}\|u\|_{L^{3/2,1}}$ by (2-39), we obtain that

$$\|(X_2(t)+X_3(t)-S(t))u\|_{L^\infty} \lesssim t^{-\frac{3}{2}}\|u\|_{L^1}, \quad \|(X_2(t)+X_3(t)-S(t))u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}}\|u\|_{L^{3/2,1}}. \tag{2-43}$$

Recall that

$$e^{-itH}P_c = Z_1(t)+Z_2(t)+X_2(t)+X_3(t) = Z(t)+R(t)+S(t).$$

We obtain for $Z(t) = Z_1(t) + (Z_2(t) - R(t)) + (X_2(t) + X_3(t) - S(t))$ that

$$\|Z(t)u\|_{L^\infty} \lesssim t^{-\frac{3}{2}}\|u\|_{L^1}, \quad \|Z(t)u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}}\|u\|_{L^{3/2,1}}.$$

Conclusion (2-40) follows by interpolation.

Finally, assume that all the eigenfunctions ϕ_k are in L^1 for $2 \le k \le N$ (recall that ϕ_1 is the resonance). Then, by Lemma 2.5, it follows that $\langle V\phi_k, y_\ell\rangle = \langle V\phi_k, y_\ell y_m\rangle = 0$ for all ℓ and m and all $2 \le k \le N$. As a consequence, we immediately see that

$$P_0 V|x-y|^2 V P_0 = P_0 V(|x|^2 + |y|^2) P_0 - 2\sum_{k=1}^{3} P_0 V x_k y_k V P_0 = 0.$$

Since $\langle \phi_k, V\rangle = 0$ and $\langle V\phi_k, y_\ell\rangle = 0$, we can also rewrite

$$\mu_t(x)|x-y|VP_0 = \mu_t(x)\biggl(|x-y| - |x| + \frac{xy}{|x|}\biggr)VP_0.$$

Then note that $|x|\bigl(|x-y| - |x| + \frac{xy}{|x|}\bigr)VP_0$ is bounded in absolute value by

$$\sum_{k=2}^{N} \int_{\mathbb{R}^3} |y|^2 |V(y)|\,|\phi_k(y)|\,dy \otimes |\phi_k(z)|,$$

which is bounded from L^1 to L^∞ since $\phi_k \in \langle x\rangle^{-2} L^\infty$ and $V \in \langle x\rangle^{-1} L^{\frac{3}{2},1}$. Having gained a power of decay in x, we use it by $\bigl|\mu_t(x)|x|^{-1}\bigr| \lesssim t^{-1}$. Therefore,

$$\bigl\|t^{-\frac{1}{2}}\mu_t(x)|x-y|VP_0 u\bigr\|_{L^\infty} \lesssim t^{-\frac{3}{2}}\|u\|_{L^1}.$$

Consequently, when $\phi_k \in L^1$ for $2 \le k \le N$, we can remove $S(t)$ from (2-43). Hence we retrieve conclusion (2-40) without S, as claimed. □

Proposition 2.19. *Assume that $V \in \langle x\rangle^{-2} L^{\frac{3}{2},1}$ and that $H = -\Delta + V$ is an exceptional Hamiltonian of the third kind. Then*

$$\|e^{-itH} P_c u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}} \|u\|_{L^{3/2,1}}$$

and, for $\frac{3}{2} < p \le 2$,

$$\|e^{-itH} P_c u\|_{L^{p'}} \lesssim t^{-\frac{3}{2}\left(\frac{1}{p} - \frac{1}{p'}\right)} \|u\|_{L^p}.$$

Here $\frac{1}{p} + \frac{1}{p'} = 1$.

The proof of this proposition parallels the proof of Proposition 2.15.

Proof of Proposition 2.19. Write the evolution as

$$e^{-itH} P_c f = \frac{1}{i\pi}\int_{\mathbb{R}} e^{-it\lambda^2}\bigl(R_0((\lambda+i0)^2) - R_0((\lambda+i0)^2) V_1 \widehat{T}(\lambda)^{-1} V_2 R_0((\lambda+i0)^2)\bigr) f \lambda\, d\lambda.$$

We consider a partition of unity subordinated to the neighborhoods of Lemmas 2.8 and 2.17. First, take a sufficiently large R such that

$$\Bigl(1 - \chi\Bigl(\frac{\lambda}{R}\Bigr)\Bigr)(I + \widehat{T}(\lambda))^{-1} \in \mathcal{W}.$$

Then, for every $\lambda_0 \in [-4R, 4R]$, there exists $\epsilon(\lambda_0) > 0$ such that

$$\chi\Big(\frac{\lambda-\lambda_0}{\epsilon(\lambda_0)}\Big)(I+\widehat{T}(\lambda))^{-1} \in \mathcal{W}$$

if $\lambda_0 \neq 0$, while the conclusion of Lemma 2.12 holds when $\lambda_0 = 0$.

Since $[-4R, 4R]$ is a compact set, there exists a finite covering

$$[-4R, 4R] \subset \bigcup_{k=1}^{N} \big(\lambda_k - \epsilon(\lambda_k), \lambda_k + \epsilon(\lambda_k)\big).$$

Then we construct a finite partition of unity on $\mathbb{R}$ by smooth functions $1 = \chi_0(\lambda) + \sum_{k=1}^{N} \chi_k(\lambda) + \chi_\infty(\lambda)$, where $\operatorname{supp} \chi_\infty \subset \mathbb{R} \setminus (-2R, 2R)$, $\operatorname{supp} \chi_0 \subset [-\epsilon(0), \epsilon(0)]$, and $\operatorname{supp} \chi_k \subset \big[\lambda_k - \epsilon(\lambda_k), \lambda_k + \epsilon(\lambda_k)\big]$.

By Lemma 2.8, for any $k \neq 0$, we have $\chi_k(\lambda)(I+\widehat{T}(\lambda))^{-1} \in \mathcal{W}$, so $(1-\chi_0(\lambda))(I+\widehat{T}(\lambda))^{-1} \in \mathcal{W}$. By Lemma 2.17,

$$\chi_0(\lambda)(I+\widehat{T}(\lambda))^{-1} = L(\lambda) + \lambda^{-1} S(\lambda) + \lambda^{-2} V_2 P_0 V_1,$$

where $L \in \mathcal{W}$ and $S^\vee \in \mathcal{V}_{L^{3,2}, L^{3/2,2}}$.

Let Z_1 be given by the sum of all the regular terms of the decomposition:

$$\begin{aligned}
Z_1(t) &:= \frac{1}{i\pi} \int_{\mathbb{R}} e^{-it\lambda^2} \big(R_0((\lambda+i0)^2) - R_0((\lambda+i0)^2) V_1 L(\lambda) V_2 R_0((\lambda+i0)^2) \\
&\qquad - (1-\chi_0(\lambda)) R_0((\lambda+i0)^2) V_1 \widehat{T}(\lambda) V_2 R_0((\lambda+i0)^2)\big) \lambda \, d\lambda \\
&= \frac{1}{2\pi t} \int_{\mathbb{R}} e^{-it\lambda^2} \partial_\lambda \big(R_0((\lambda+i0)^2) - R_0((\lambda+i0)^2) V_1 L(\lambda) V_2 R_0((\lambda+i0)^2) \\
&\qquad - (1-\chi_0(\lambda)) R_0((\lambda+i0)^2) V_1 \widehat{T}(\lambda) V_2 R_0((\lambda+i0)^2)\big) \, d\lambda \\
&= \frac{C}{t^{\frac{3}{2}}} \int_{\mathbb{R}} e^{-i\frac{\rho^2}{4t}} \big(\partial_\lambda \big(R_0((\lambda+i0)^2) - R_0((\lambda+i0)^2) V_1 L(\lambda) V_2 R_0((\lambda+i0)^2) \\
&\qquad - (1-\chi_0(\lambda)) R_0((\lambda+i0)^2) V_1 \widehat{T}(\lambda) V_2 R_0((\lambda+i0)^2)\big)\big)^\vee(\rho) \, d\rho.
\end{aligned}$$

The fact that $\|Z_1(t)u\|_{L^\infty} \lesssim |t|^{-\frac{3}{2}} \|u\|_{L^1}$ follows by knowing that

$$\begin{aligned}
&\big(\partial_\lambda \big(R_0((\lambda+i0)^2) - R_0((\lambda+i0)^2) V_1 L(\lambda) V_2 R_0((\lambda+i0)^2) \\
&\qquad - (1-\chi_0(\lambda)) R_0((\lambda+i0)^2) V_1 \widehat{T}(\lambda) V_2 R_0((\lambda+i0)^2)\big)\big)^\vee \in \mathcal{V}_{L^1, L^\infty}.
\end{aligned}$$

Using smoothing estimates, it immediately follows that $Z_1(t)$ is L^2-bounded; see the proof of Proposition 2.13. Interpolating, we obtain that $\|Z_1(t)u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}} \|u\|_{L^{3,1}}$.

Let Z_2 be the following singular term in the decomposition of Lemma 2.17:

$$\begin{aligned}
Z_2(t) &:= \frac{1}{i\pi} \int_{\mathbb{R}} e^{-it\lambda^2} R_0((\lambda+i0)^2) V_1 S(\lambda) V_2 R_0((\lambda+i0)^2) \, d\lambda \\
&= \frac{C}{t^{\frac{1}{2}}} \int_{\mathbb{R}} e^{-i\frac{\rho^2}{4t}} \big(R_0((\lambda+i0)^2) V_1 S(\lambda) V_2 R_0((\lambda+i0)^2)\big)^\vee(\rho) \, d\rho.
\end{aligned}$$

Note that

$$\big(R_0((\lambda+i0)^2)V_1\big)^\vee \in \mathcal{V}_{L^{3/2,2},L^{3,\infty}}, \quad S(\lambda)^\vee \in \mathcal{V}_{L^{3,2},L^{3/2,2}} \quad \text{and} \quad (V_2 R_0((\lambda+i0)^2))^\vee \in \mathcal{V}_{L^{3/2,1},L^{3,2}}.$$

Thus

$$R_0((\lambda+i0)^2)V_1(\lambda S(\lambda))V_2 R_0((\lambda+i0)^2) \in \mathcal{V}_{L^{3/2,1},L^{3,\infty}}.$$

This immediately implies that $\|Z_2(t)u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}}\|u\|_{L^{3/2,1}}$.

We are left with the contribution of the term $\lambda^{-2}V_2P_0V_1$. This is the same as the term X_3 from the proof of Proposition 2.18. By (2-42), we have $\|X_3(t)u\|_{L^{3,\infty}} \lesssim t^{-\frac{1}{2}}\|u\|_{L^{3/2,1}}$.

Putting the three estimates for Z_1, Z_2, and X_3 together, we obtain that $\|e^{-itH}P_c u\|_{L^{3,\infty}} \lesssim \|u\|_{L^{3/2,1}}$. Interpolating with the obvious L^2 bound $\|e^{-itH}P_c u\|_{L^2} \lesssim \|u\|_{L^2}$, we obtain the stated conclusion. □

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References

[Beceanu 2011] M. Beceanu, "New estimates for a time-dependent Schrödinger equation", *Duke Math. J.* **159**:3 (2011), 417–477. MR 2831875 Zbl 1229.35224

[Beceanu and Goldberg 2012] M. Beceanu and M. Goldberg, "Schrödinger dispersive estimates for a scaling-critical class of potentials", *Comm. Math. Phys.* **314**:2 (2012), 471–481. MR 2958960 Zbl 1250.35047

[Beceanu and Goldberg 2014] M. Beceanu and M. Goldberg, "Strichartz estimates and maximal operators for the wave equation in $\mathbb{R}^3$", *J. Funct. Anal.* **266**:3 (2014), 1476–1510. MR 3146823 Zbl 1292.35063

[Bergh and Löfström 1976] J. Bergh and J. Löfström, *Interpolation spaces: An introduction*, Grundlehren der Mathematischen Wissenschaften **223**, Springer, Berlin, 1976. MR 0482275 Zbl 0344.46071

[Cardoso et al. 2009] F. Cardoso, C. Cuevas, and G. Vodev, "Dispersive estimates for the Schrödinger equation in dimensions four and five", *Asymptot. Anal.* **62**:3-4 (2009), 125–145. MR 2521760 Zbl 1163.35482

[Egorova et al. 2014] I. Egorova, E. Kopylova, V. Marchenko, and G. Teschl, "Dispersion estimates for one-dimensional Schrödinger and Klein-Gordon equations revisited", preprint, 2014. To appear in *Russian Math. Surveys*. arXiv 1411.0021

[Erdoğan and Green 2010] M. B. Erdoğan and W. R. Green, "Dispersive estimates for the Schrödinger equation for $C^{\frac{n-3}{2}}$ potentials in odd dimensions", *Int. Math. Res. Not.* **2010**:13 (2010), 2532–2565. MR 2669658 Zbl 1200.35036

[Erdoğan and Green 2013a] M. B. Erdoğan and W. R. Green, "Dispersive estimates for matrix Schrödinger operators in dimension two", *Discrete Contin. Dyn. Syst.* **33**:10 (2013), 4473–4495. MR 3049087 Zbl 1277.35294

[Erdoğan and Green 2013b] M. B. Erdoğan and W. R. Green, "Dispersive estimates for Schrödinger operators in dimension two with obstructions at zero energy", *Trans. Amer. Math. Soc.* **365**:12 (2013), 6403–6440. MR 3105757 Zbl 1282.35143

[Erdoğan and Green 2013c] M. B. Erdoğan and W. R. Green, "A weighted dispersive estimate for Schrödinger operators in dimension two", *Comm. Math. Phys.* **319**:3 (2013), 791–811. MR 3040376 Zbl 1272.35053

[Erdoğan and Schlag 2004] M. B. Erdoğan and W. Schlag, "Dispersive estimates for Schrödinger operators in the presence of a resonance and/or an eigenvalue at zero energy in dimension three, I", *Dyn. Partial Differ. Equ.* **1**:4 (2004), 359–379. MR 2127577 Zbl 1080.35102

[Erdoğan and Schlag 2006] M. B. Erdoğan and W. Schlag, "Dispersive estimates for Schrödinger operators in the presence of a resonance and/or an eigenvalue at zero energy in dimension three, II", *J. Anal. Math.* **99** (2006), 199–248. MR 2279551 Zbl 1146.35324

[Erdoğan et al. 2014] M. B. Erdoğan, M. Goldberg, and W. R. Green, "Dispersive estimates for four dimensional Schrödinger and wave equations with obstructions at zero energy", *Comm. Partial Differential Equations* **39**:10 (2014), 1936–1964. MR 3250981 Zbl 1325.35017

[Goldberg 2006] M. Goldberg, "Dispersive bounds for the three-dimensional Schrödinger equation with almost critical potentials", *Geom. Funct. Anal.* **16**:3 (2006), 517–536. MR 2238943 Zbl 1158.35408

[Goldberg 2007] M. Goldberg, "Transport in the one-dimensional Schrödinger equation", *Proc. Amer. Math. Soc.* **135**:10 (2007), 3171–3179. MR 2322747 Zbl 1123.35046

[Goldberg 2010] M. Goldberg, "A dispersive bound for three-dimensional Schrödinger operators with zero energy eigenvalues", *Comm. Partial Differential Equations* **35**:9 (2010), 1610–1634. MR 2754057 Zbl 1223.35265

[Goldberg and Green 2014] M. Goldberg and W. R. Green, "Dispersive estimates for higher dimensional Schrödinger operators with threshold eigenvalues, II: The even dimensional case", preprint, 2014. To appear in *J. Spectr. Theory*. arXiv 1409.6328

[Goldberg and Green 2015] M. Goldberg and W. R. Green, "Dispersive estimates for higher dimensional Schrödinger operators with threshold eigenvalues, I: The odd dimensional case", *J. Funct. Anal.* **269**:3 (2015), 633–682. MR 3350725 Zbl 1317.35216

[Goldberg and Schlag 2004a] M. Goldberg and W. Schlag, "Dispersive estimates for Schrödinger operators in dimensions one and three", *Comm. Math. Phys.* **251**:1 (2004), 157–178. MR 2096737 Zbl 1086.81077

[Goldberg and Schlag 2004b] M. Goldberg and W. Schlag, "A limiting absorption principle for the three-dimensional Schrödinger equation with L^p potentials", *Int. Math. Res. Not.* **2004**:75 (2004), 4049–4071. MR 2112327 Zbl 1069.35063

[Green 2012] W. R. Green, "Dispersive estimates for matrix and scalar Schrödinger operators in dimension five", *Illinois J. Math.* **56**:2 (2012), 307–341. MR 3161326 Zbl 06233916

[Ionescu and Jerison 2003] A. D. Ionescu and D. Jerison, "On the absence of positive eigenvalues of Schrödinger operators with rough potentials", *Geom. Funct. Anal.* **13**:5 (2003), 1029–1081. MR 2024415 Zbl 1055.35098

[Jensen and Kato 1979] A. Jensen and T. Kato, "Spectral properties of Schrödinger operators and time-decay of the wave functions", *Duke Math. J.* **46**:3 (1979), 583–611. MR 544248 Zbl 0448.35080

[Jensen and Nenciu 2001] A. Jensen and G. Nenciu, "A unified approach to resolvent expansions at thresholds", *Rev. Math. Phys.* **13**:6 (2001), 717–754. MR 1841744 Zbl 1029.81067

[Journé et al. 1991] J.-L. Journé, A. Soffer, and C. D. Sogge, "Decay estimates for Schrödinger operators", *Comm. Pure Appl. Math.* **44**:5 (1991), 573–604. MR 1105875 Zbl 0743.35008

[Murata 1982] M. Murata, "Asymptotic expansions in time for solutions of Schrödinger-type equations", *J. Funct. Anal.* **49**:1 (1982), 10–56. MR 680855 Zbl 0499.35019

[Rauch 1978] J. Rauch, "Local decay of scattering solutions to Schrödinger's equation", *Comm. Math. Phys.* **61**:2 (1978), 149–168. MR 0495958 Zbl 0381.35023

[Schlag 2005] W. Schlag, "Dispersive estimates for Schrödinger operators in dimension two", *Comm. Math. Phys.* **257**:1 (2005), 87–117. MR 2163570 Zbl 1134.35321

[Simon 1982] B. Simon, "Schrödinger semigroups", *Bull. Amer. Math. Soc.* (*N.S.*) **7**:3 (1982), 447–526. MR 670130 Zbl 0524.35002

[Stein 1993] E. M. Stein, *Harmonic analysis: real-variable methods, orthogonality, and oscillatory integrals*, Princeton Mathematical Series **43**, Princeton University Press, 1993. MR 1232192 Zbl 0821.42001

[Yajima 2005] K. Yajima, "Dispersive estimates for Schrödinger equations with threshold resonance and eigenvalue", *Comm. Math. Phys.* **259**:2 (2005), 475–509. MR 2172692 Zbl 1079.81021

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INTERIOR NODAL SETS OF STEKLOV EIGENFUNCTIONS ON SURFACES

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We investigate the interior nodal sets $\mathcal{N}_\lambda$ of Steklov eigenfunctions on connected and compact surfaces with boundary. The optimal vanishing order of Steklov eigenfunctions is shown be $C\lambda$. The singular sets $\mathcal{S}_\lambda$ consist of finitely many points on the nodal sets. We are able to prove that the Hausdorff measure $H^0(\mathcal{S}_\lambda)$ is at most $C\lambda^2$. Furthermore, we obtain an upper bound for the measure of interior nodal sets, $H^1(\mathcal{N}_\lambda) \le C\lambda^{3/2}$. Here the positive constants C depend only on the surfaces.

1. Introduction

Let $(\mathcal{M}, g)$ be a smooth, connected and compact surface with smooth boundary $\partial\mathcal{M}$. The main goal of this paper is to obtain an upper bound of interior nodal sets

$$\mathcal{N}_\lambda = \{z \in \mathcal{M} \mid e_\lambda = 0\}$$

for Steklov eigenfunctions, which satisfy

$$\begin{cases} \triangle_g e_\lambda = 0, & z \in \mathcal{M}, \\ \partial e_\lambda(z)/\partial \nu = \lambda e_\lambda(z), & z \in \partial\mathcal{M}, \end{cases} \tag{1-1}$$

where ν is a unit outward normal on $\partial\mathcal{M}$. The Steklov eigenfunctions were introduced by Steklov in 1902 for bounded domains in the plane. They interpret the steady state temperature distribution in domains where the heat flux on the boundary is proportional to the temperature. They also have applications in quite a few physical fields, such as fluid mechanics, electromagnetism and elasticity. In particular, the model (1-1) was studied by Calderón [1980] as solutions can be regarded as eigenfunctions of the Dirichlet-to-Neumann map. The interior nodal sets of Steklov eigenfunctions represent the stationary points in $\mathcal{M}$. In the context of quantum mechanics, nodal sets are the sets where a free particle is least likely to be found.

It is well known that the spectrum λ_j of the Steklov eigenvalue problem is discrete with

$$0 = \lambda_0 < \lambda_1 \le \lambda_2 \le \lambda_3 \le \cdots \quad \text{and} \quad \lim_{j\to\infty} \lambda_j = \infty.$$

There exists an orthonormal basis $\{e_{\lambda_j}\}$ of eigenfunctions such that

$$e_{\lambda_j} \in C^\infty(\mathcal{M}) \quad \text{and} \quad \int_{\partial\mathcal{M}} e_{\lambda_j} e_{\lambda_k} \, dV_g = \delta_j^k.$$

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Estimating the Hausdorff measure of nodal sets has always been an important subject concerning the study of eigenfunctions. This subject centers around the famous Yau conjecture. Recently, much work has been devoted to the bounds of nodal sets

$$Z_\lambda = \{z \in \partial \mathcal{M} \mid e_\lambda(z) = 0\}$$

of Steklov eigenfunctions on the boundary. Bellová and Lin [2015] proved $H^{m-1}(Z_\lambda) \leq C\lambda^6$ with C depending only on $\mathcal{M}$ if $\mathcal{M}$ is an $m+1$-dimensional analytic manifold. Zelditch [2014] improved their results and gave the optimal upper bound $H^{m-1}(Z_\lambda) \leq C\lambda$ for analytic manifolds using microlocal analysis. For the smooth manifold $\mathcal{M}$, Wang and Zhu [2015] recently established a lower bound

$$H^{m-1}(Z_\lambda) \geq C\lambda^{(3-m)/2}.$$

Before presenting our results for interior nodal sets, let's briefly review the literature about the nodal sets of classical eigenfunctions. The interested reader may refer to the book [Han and Lin 2008] and survey [Zelditch 2008] for detailed accounts about this subject. Let e_λ be L^2 normalized eigenfunctions of the Laplace–Beltrami operator on compact manifolds $(\mathcal{M}, g)$ without boundary,

$$-\triangle_g e_\lambda = \lambda^2 e_\lambda. \tag{1-2}$$

Yau's conjecture states that, for any smooth manifolds, one should control the upper and lower bounds of nodal sets of classical eigenfunctions as

$$c\lambda \leq H^{n-1}(\mathcal{N}_\lambda) \leq C\lambda, \tag{1-3}$$

where C and c depend only on the manifold $\mathcal{M}$. The conjecture is only verified for real analytic manifolds, by Donnelly and Fefferman [1988]. Lin [1991] also showed the upper bound for analytic manifolds by a different approach. For smooth manifolds, the conjecture is still not settled. For the lower bound of nodal sets with $n \geq 3$, Colding and Minicozzi [2011] and Sogge and Zelditch [2011; 2012] independently obtained that

$$H^{n-1}(\mathcal{N}_\lambda) \geq C\lambda^{(3-n)/2}$$

for smooth manifolds. See also [Hezari and Sogge 2012] for deriving the same bound by adapting the idea in [Sogge and Zelditch 2011]. For the upper bound, Hardt and Simon [1989] gave an exponential upper bound

$$H^{n-1}(\mathcal{N}_\lambda) \leq Ce^{\lambda \ln \lambda}.$$

In surfaces, better results have been obtained. Brüning [1978] and Yau (unpublished) derived the same lower bound as (1-3). The best estimate to date for the upper bound is

$$H^1(\mathcal{N}_\lambda) \leq C\lambda^{3/2}$$

by Donnelly and Fefferman [1990a] and Dong [1992] using different methods.

Let us return to the Steklov eigenvalue problem (1-1). By the maximum principle, there exist nodal sets in the manifold $\mathcal{M}$ and those sets must intersect the boundary $\partial\mathcal{M}$. Thus it is natural to study the size of interior nodal sets in $\mathcal{M}$. We can also ask Yau-type questions about the Hausdorff measure of nodal sets. The natural and corresponding conjecture for Steklov eigenfunctions should be exactly the same as (1-3). See also the open questions in the survey by Girouard and Polterovich [2014]. Recently, Sogge, Wang and the author [Sogge et al. 2015] obtained a lower bound for interior nodal sets

$$H^{n-1}(\mathcal{N}_\lambda) \geq C\lambda^{(2-n)/2}$$

for n-dimensional manifolds $\mathcal{M}$. Very recently, Polterovich, Sher and Toth [Polterovich et al. 2015] verified the Yau-type conjecture for (1-1) on real analytic Riemannian surfaces.

An interesting topic related to the measure of nodal sets is about doubling inequalities. Based on doubling inequalities, one can obtain the vanishing order of eigenfunctions, which characterizes how fast the eigenfunctions vanish. For the classical eigenfunctions of (1-2), Donnelly and Fefferman [1988; 1990b] obtained that the maximal vanishing order of e_λ is of order at most $C\lambda$ everywhere. To achieve it, a doubling inequality

$$\int_{\mathbb{B}(z_0,2r)} e_\lambda^2 \leq Ce^\lambda \int_{\mathbb{B}(z_0,r)} e_\lambda^2 \tag{1-4}$$

is derived using Carleman estimates, where $\mathbb{B}(p, c)$ denotes a ball centered at p with radius c. The doubling estimate (1-4) plays an important role in obtaining the bounds of nodal sets for analytic manifolds in [Donnelly and Fefferman 1988] and the upper bound of nodal sets for smooth surfaces in [Donnelly and Fefferman 1990a]. For the Steklov eigenfunctions, we obtain a doubling inequality on the boundary $\partial\mathcal{M}$ and derive that the sharp vanishing order is less than $C\lambda$ on the boundary $\partial\mathcal{M}$. For Steklov eigenfunctions in $\mathcal{M}$, we are also able to get the doubling inequality; see Proposition 5. With the aid of doubling estimates and Carleman inequalities, the following optimal vanishing order for Steklov eigenfunctions can be obtained:

Theorem 1. *The vanishing order of the Steklov eigenfunction e_λ of* (1-1) *in $\mathcal{M}$ is everywhere less than $C\lambda$.*

Its sharpness can be seen in the case that the manifold $\mathcal{M}$ is a ball. Notice that the doubling estimates in Proposition 5 and the vanishing order in Theorem 1 hold for any n-dimensional compact manifolds.

Singular sets

$$\mathcal{S}_\lambda = \{z \in \mathcal{M} \mid e_\lambda = 0,\ \nabla e_\lambda = 0\}$$

are contained in nodal sets. In Riemannian surfaces, those singular sets consist of finitely many points in the 1-dimensional nodal sets. It is interesting to count the number of those singular sets. Based on a Carleman inequality with singularities, we are able to show an upper bound of singular sets.

Theorem 2. *Let $(\mathcal{M}, g)$ be a smooth, connected and compact surface with smooth boundary $\partial\mathcal{M}$. Then*

$$H^0(\mathcal{S}_\lambda) \leq C\lambda^2 \tag{1-5}$$

holds for Steklov eigenfunctions in (1-1).

For the nodal sets of Steklov eigenfunctions, we are able to build a similar type of Carleman inequality as [Donnelly and Fefferman 1990a], and show the following result:

Theorem 3. *Let* $(\mathcal{M}, g)$ *be a smooth, connected and compact surface with smooth boundary* $\partial\mathcal{M}$*. Then*

$$H^1(\mathcal{N}_\lambda) \le C\lambda^{3/2} \tag{1-6}$$

holds for Steklov eigenfunctions in (1-1).

The outline of the paper is as follows. Section 2 is devoted to reducing the Steklov eigenvalue problem into an equivalent elliptic equation without boundary. Then we obtain the optimal doubling inequality and show Theorem 1. In Section 3, we establish the Carleman inequality with singularities at finitely many points. Under additional assumptions on those singular points, a stronger Carleman inequality is derived. We measure the singular sets in Section 4. Sections 5, 6 and 7 are devoted to obtaining the nodal length of Steklov eigenfunctions. Under the condition of slow growth of L^2 norm, we find out the nodal length in Section 6. Based on a similar type of Calderón and Zygmund decomposition procedure, we show the slow growth at almost every point. Then the measure of nodal sets is derived by summing up the nodal length in each small square. The letters c, C, C_i, d_i denote generic positive constants and do not depend on λ. They may vary in different lines and sections.

2. Vanishing order of Steklov eigenfunctions

In this section, we will reduce the Steklov eigenvalue problem to an equivalent model on a boundaryless manifold. The presence of eigenvalues on the boundary $\partial\mathcal{M}$ will be reflected in the coefficient functions of a second-order elliptic equation. Let $d(z) = \text{dist}\{z, \partial\mathcal{M}\}$ denote the geodesic distance function from $x \in \mathcal{M}$ to the boundary $\partial\mathcal{M}$. Since $\mathcal{M}$ is smooth, there exists a ρ-neighborhood of $\partial\mathcal{M}$ in $\mathcal{M}$ such that $d(x)$ is smooth in the neighborhood. Let's denote it as $\mathcal{M}_\rho$. We extend $d(z)$ smoothly in $\mathcal{M}$ by

$$\delta(z) = \begin{cases} d(z), & z \in \mathcal{M}_\rho, \\ l(z), & z \in \mathcal{M}\backslash\mathcal{M}_\rho, \end{cases} \tag{2-1}$$

where $l(z)$ is a smooth function in $\mathcal{M}\backslash\mathcal{M}_\rho$. Note that the extended function $\delta(z)$ is a smooth function in $\mathcal{M}$. We first reduce the Steklov eigenvalue problem into an elliptic equation with Neumann boundary condition. Let

$$v(z) = e_\lambda \exp\{\lambda\delta(z)\}.$$

It is known that $v(z) = e_\lambda(z)$ on $\partial\mathcal{M}$. For $z \in \partial\mathcal{M}$, we have $\nabla_g\delta(z) = -\nu(z)$. Recall that $\nu(z)$ is the unit outer normal on $z \in \partial\mathcal{M}$. We can check that the new function $v(z)$ satisfies

$$\begin{cases} \triangle_g v + b(z)\cdot\nabla_g v + q(z)v = 0 & \text{in } \mathcal{M}, \\ \partial v/\partial\nu = 0 & \text{on } \partial\mathcal{M}, \end{cases} \tag{2-2}$$

with

$$\begin{cases} b(z) = -2\lambda\nabla_g\delta(z), \\ q(z) = \lambda^2|\nabla_g\delta(z)|^2 - \lambda\triangle_g\delta(z). \end{cases} \tag{2-3}$$

In order to get rid of the boundary condition, we attach two copies of $\mathcal{M}$ along the boundary and consider the double manifold $\bar{\mathcal{M}} = \mathcal{M}\cup\mathcal{M}$. The metric g extends to $\bar{\mathcal{M}}$ with Lipschitz-type singularity along $\partial\mathcal{M}$, since the lift metric g' of g on $\mathcal{M}$ to the double manifold $\bar{\mathcal{M}}$ is Lipschitz. There also exists a canonical involutive isometry $\mathcal{F}:\bar{\mathcal{M}}\to\bar{\mathcal{M}}$ that interchanges the two copies of $\mathcal{M}$. Then the function $v(x)$ can be extended to $\bar{\mathcal{M}}$ by $v\circ\mathcal{F}=v$. Therefore, $v(z)$ satisfies

$$\triangle_{g'}v+\bar{b}(z)\cdot\nabla_{g'}v+\bar{q}(z)v=0 \quad \text{in } \bar{\mathcal{M}}. \tag{2-4}$$

From (2-3), one can see that

$$\begin{cases}\|\bar{b}\|_{W^{1,\infty}(\bar{\mathcal{M}})}\le C\lambda,\\ \|\bar{q}\|_{W^{1,\infty}(\bar{\mathcal{M}})}\le C\lambda^2.\end{cases} \tag{2-5}$$

After this procedure, we can instead study the nodal sets for the second-order elliptic equation (2-4) with assumption (2-5). Note that $\bar{\mathcal{M}}$ is a manifold without boundary.

We present a brief proof of Theorem 1. It is a small modification of the argument in [Zhu 2015], where the sharp vanishing order of Steklov eigenfunctions on the boundary $\partial\mathcal{M}$ is shown to be less than $C\lambda$. To achieve it, we derive the double inequality in a neighborhood of the boundary by quantitative Carleman estimates.

Proof of Theorem 1. Recall the strategy in [Zhu 2015]; we do an even reflection in a small neighborhood of the boundary. Then we deal with a second-order elliptic equation with a Lipschitz-continuous leading coefficient function and satisfying the same conditions as (2-5). By the regularity argument for dealing with a Lipschitz metric in [Donnelly and Fefferman 1990b], the same Carleman estimates in [Zhu 2015] hold for (2-4). Let $r(z)$ be the distance function from z to the fixed point z_0. If $u\in C_0^\infty(\mathbb{B}_{r_0}(z_0)\backslash\{z_0\})$ and $\tau>C_1(1+\|\bar{b}\|_{W^{1,\infty}}+\|\bar{q}\|_{W^{1,\infty}}^{1/2})$, following the arguments in [Zhu 2015] and choosing the test function $\tilde{\phi}(z)=\ln r(z)-r^\epsilon(z)$ there instead, we have the Carleman inequality

$$C\|r^2e^{\tau\phi(r)}(\triangle_{g'}u+\bar{b}\cdot\nabla_{g'}u+\bar{q}u)\|_{L^2}\ge\tau^{3/2}\|r^{\epsilon/2}e^{\tau\phi(r)}u\|_{L^2}+\tau^{1/2}\|r^{1+\epsilon/2}e^{\tau\phi(r)}\nabla u\|_{L^2},$$

where $\phi(r)=-\ln r(z)+r^\epsilon(z)$. See also, e.g., [Bakri and Casteras 2014] for similar estimates on manifolds with smooth metric. In particular, we have the following lemma:

Lemma 4. *Let $u\in C_0^\infty\big(\tfrac{1}{2}\epsilon_1<r<\epsilon_0\big)$. If $\tau>C_1(1+\|\bar{b}\|_{W^{1,\infty}}+\|\bar{q}\|_{W^{1,\infty}}^{1/2})$. Then*

$$\int r^4e^{2\tau\phi(r)}|\triangle_{g'}u+\bar{b}\cdot\nabla_{g'}u+\bar{q}u|^2\,dr\,d\omega\ge C_2\tau^3\int r^\epsilon e^{2\tau\phi(r)}u^2\,dr\,d\omega, \tag{2-6}$$

where $\phi(r)=-\ln r(z)+r^\epsilon(z)$ and $0<\epsilon_0,\epsilon_1,\epsilon<1$ are some fixed constants. Moreover, (r,ω) are the standard polar coordinates.

Using this Carleman estimate and choosing suitable test functions, a Hadamard three-ball result can be obtained in $\bar{\mathcal{M}}$ following the arguments in [Zhu 2015]. There exist constants r_0, C and $0<\gamma<1$ depending only on $\bar{\mathcal{M}}$ such that, for any solutions of (2-4), $0<r<r_0$ and $z_0\in\bar{\mathcal{M}}$, one has

$$\int_{\mathbb{B}(z_0,r)}v^2\le e^{C(1+\|\bar{b}\|_{W^{1,\infty}}+\|\bar{q}\|_{W^{1,\infty}}^{1/2})}\bigg(\int_{\mathbb{B}(z_0,2r)}v^2\bigg)^{1-\gamma}\bigg(\int_{\mathbb{B}(z_0,r/2)}v^2\bigg)^{\gamma}. \tag{2-7}$$

Based on a propagation of smallness argument using the three-ball result and Carleman estimates (2-6), as that in [Zhu 2015], taking the assumptions (2-5) into account, we are able to obtain the doubling inequality in $\bar{\mathcal{M}}$.

Proposition 5. *There exist constants r_0 and C depending only on $\bar{\mathcal{M}}$ such that, for any $0 < r < r_0$ and $z_0 \in \bar{\mathcal{M}}$,*

$$\|v\|_{L^2(\mathbb{B}(z_0,2r))} \leq e^{C\lambda} \|v\|_{L^2(\mathbb{B}(z_0,r))} \tag{2-8}$$

for any solutions of (2-4).

One can see that the doubling estimate holds in $\mathcal{M}$ if $\mathbb{B}(z_0, 2r) \subset \mathcal{M}$. By standard elliptic estimates, one can have the L^∞ norm doubling inequality

$$\|v\|_{L^\infty(\mathbb{B}(z_0,2r))} \leq e^{C\lambda} \|v\|_{L^\infty(\mathbb{B}(z_0,r))}.$$

Since $\bar{\mathcal{M}}$ is compact, we can derive that

$$\|v\|_{L^\infty(\mathbb{B}(z_0,r))} \geq r^{C\lambda}$$

for any $z_0 \in \bar{\mathcal{M}}$, which implies the vanishing order for v is less than $C\lambda$. So is the vanishing order of u. This completes Theorem 1. □

3. Carleman estimates

This section is devoted to establishing Carleman inequalities involving weighted functions at finitely many points. From this section on, $\bar{\mathcal{M}}$ is a compact Riemannian surface. We construct suitable conformal coordinate charts near $\partial\mathcal{M} \subset \bar{\mathcal{M}}$ following the arguments in [Donnelly and Fefferman 1990a, p. 342–343], where the same construction is established for a Lipschitz double manifold. By the Riemann mapping theory in [Jost 1984], we first construct charts around $\partial\mathcal{M} \subset \mathcal{M}$. We map a half disk centered on the x-axis in the (x, y)-plane into the manifold $\mathcal{M}$ with the x-axis mapped to $\partial\mathcal{M}$. Thus, the metric is locally given as $\bar{g}(x, y)(dx^2 + dy^2)$ with $y > 0$. The differentiable structure and the definition of the metric on the double manifold $\bar{\mathcal{M}}$ correspond to reflection about the x-axis. Thus, we have the required the conformal charts with $\bar{g}(x, |y|)(dx^2 + dy^2)$ on the double manifold $\bar{\mathcal{M}}$. Then we will consider the behavior of v in a conformal coordinate patch. There exists a finite number N of conformal charts $(\mathcal{U}_i, \phi_i)$ with $\phi_i : \mathcal{U}_i \subset \bar{\mathcal{M}} \to \mathcal{V}_i \subset \mathbb{R}^2$ and $i \in \{1, 2, \ldots, N\}$. On each of these charts, the metric is conformally flat and there exists a positive function g_i such that $g' = g_i(x, y)(dx^2 + dy^2)$. By the compactness of the surface, there are positive constants c and C such that $0 < c < g_i < C$ for each i. Under this equivalent metric, $\triangle_{g'} = g_i^{-1}\triangle$, where $\triangle$ is the Euclidean Laplacian. Hence, (2-4) can be written as

$$\triangle v + \bar{b}(z) \cdot \nabla v + \bar{q}(z) v = 0 \quad \text{in } \mathcal{V}_i, \tag{3-1}$$

where ∇ is the Euclidean gradient and $z = (x, y)$. We use the same notations $\bar{b}(z)$ and $\bar{q}(z)$ as in (3-1), since they satisfy the same conditions as (2-5). They only differ by some function about g_i.

By restricting to a small ball $\mathbb{B}(p, 3c)$ contained in the conformal chart, we consider v in the small ball. Let $\bar{v}(z) = v(cz)$. It follows from (3-1) that

$$\triangle \bar{v} + \tilde{b}(z) \cdot \nabla \bar{v} + \tilde{q}(z) \bar{v} = 0 \quad \text{in } \mathbb{B}_3, \tag{3-2}$$

with $\tilde{b} = c\bar{b}$ and $\tilde{q} = c^2\bar{q}$. If c is sufficiently small, $\tilde{b}$ and $\tilde{q}$ are arbitrarily small.

The crucial tool in [Donnelly and Fefferman 1990a] is a Carleman inequality for classical eigenfunctions involving weighted functions with singularities at finitely many points. We will obtain the corresponding Carleman inequality for the second-order elliptic equation (3-2). We adapt the approach in [Donnelly and Fefferman 1990a] to obtain the desirable Carleman estimate for (3-2).

Let $\mathcal{D} \subset \mathcal{C}$ be an open set and $\psi \in C_0^\infty(\mathcal{D})$ be a real-valued function. We introduce the differential operators

$$\partial = \frac{1}{2}\Big(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\Big) \quad \text{and} \quad \bar\partial = \frac{1}{2}\Big(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\Big).$$

Direct computation shows that $\bar\partial\partial\psi = \frac{1}{4}\triangle\psi$. By the Cauchy–Riemann equation, u is holomorphic if and only if $\bar\partial u = 0$. For completeness, we present the elementary inequality in [Donnelly and Fefferman 1990a].

Lemma 6. *Let Φ be a smooth positive function in $\mathcal{D}$. Then*

$$\int_{\mathcal{D}} |\bar\partial u|^2 \Phi \geq \frac{1}{4}\int_{\mathcal{D}} (\triangle \ln \Phi)|u|^2\Phi. \tag{3-3}$$

Here the integral is taken with respect to the Lebesgue measure.

We want the weight function to involve those singular points. To specialize the choice of Φ, we construct the following function ψ_0:

Lemma 7. *There exists a smooth function ψ_0 defined for $|z| > 1-2a$ satisfying the following properties*:

(i) $a_1 \leq \psi_0(z) \leq a_2$ *with constants* $a_1, a_2 > 0$.

(ii) $\psi_0 = 1$ *on* $\{|z| > 1\}$.

(iii) $\triangle \ln \psi_0 \geq 0$ *on* $\{|z| > (1-2a)\}$.

(iv) *If* $1-2a < |z| < 1-a$, *then* $\triangle \ln \psi_0 \geq a_3 > 0$.

The existence of such a ψ_0 follows from existence and uniqueness theory of ordinary differential equations.

We assume that

$$D_l = \{z \mid |z-z_l| \leq \delta\}.$$

Let D_l be a finite collection of pairwise disjoint disks that are contained in a unit disk centered at the origin. Let

$$D_l(a) = \{z \mid |z-z_l| \leq (1-2a)\delta\}$$

be the smaller concentric disk. We define a smooth weight function $\Psi_0(z)$ as

$$\Psi_0(z) = \begin{cases} 1 & \text{if } z \notin \bigcup_l D_l, \\ \psi_0((z-z_l)/\delta) & \text{if } z \in D_l. \end{cases}$$

We also introduce the domain

$$A_l = \{(1-2a)\delta \leq |z-z_l| \leq (1-a)\delta\}.$$

From the last lemma, $\Psi_0(z)$ satisfies these properties:

(i) $a_1 \le \Psi_0(z) \le a_2$.

(ii) $\triangle \ln \Psi_0 \ge 0$ for $z \in \mathbb{R}^2 \setminus \bigcup_l D_l(a)$.

(iii) $\triangle \ln \Psi_0 \ge a_3 \delta^{-2}$ for $z \in A_l$.

Note that the a_i in the above are positive constants independent of λ. Let

$$A = \bigcup_l A_l.$$

Suppose that τ is a nonnegative constant. We introduce $\Phi(z) = \Psi_0(z) e^{\tau |z|^2}$. For $u \in C_0^\infty(\mathbb{R}^2 \setminus \bigcup_l D_l(a))$, we assume that $\mathfrak{D}$ contains the support of u and $A \subset \mathfrak{D} \subset \mathbb{R}^2 \setminus \cup_l D_l(a)$. Obviously,

$$\ln \Phi(z) = \ln \Psi_0(z) + \tau |z|^2.$$

Substituting Φ in Lemma 6 gives that

$$\int_{\mathfrak{D}} |\bar{\partial} u|^2 \Psi_0(z) e^{\tau |z|^2} \ge C_1 \tau \int_{\mathfrak{D}} |u|^2 \Psi_0(z) e^{\tau |z|^2} + C_2 \delta^{-2} \int_A |u|^2 e^{\tau |z|^2}, \tag{3-4}$$

where we have used the properties (ii) and (iii) for Ψ_0. The boundedness of $\Psi_0(z)$ yields that

$$\int_{\mathfrak{D}} |\bar{\partial} u|^2 e^{\tau |z|^2} \ge C_3 \tau \int_{\mathfrak{D}} |u|^2 e^{\tau |z|^2} + C_4 \delta^{-2} \int_A |u|^2 e^{\tau |z|^2}. \tag{3-5}$$

Define the holomorphic function

$$P(z) = \prod_l (z - z_l).$$

Then $\bar{\partial}(u/P) = \bar{\partial} u / P$. Replacing u by u/P in (3-5), it follows that

$$\int_{\mathfrak{D}} |\bar{\partial} u|^2 |P|^{-2} e^{\tau |z|^2} \ge C_3 \tau \int_{\mathfrak{D}} |u|^2 |P|^{-2} e^{\tau |z|^2} + C_4 \delta^{-2} \int_A |u|^2 |P|^{-2} e^{\tau |z|^2}. \tag{3-6}$$

We will establish a Carleman inequality for second-order elliptic equations like (3-2). Write $\tilde{b}(x) = (\tilde{b}_1(x), \tilde{b}_2(x))$. Let

$$u = \partial f + \tfrac{1}{2}(\tilde{b}_1 - i \tilde{b}_2) f,$$

where $f \in C_0^\infty\big(\mathbb{R}^2 \setminus \bigcup_l D_l(a)\big)$ is a real-valued function. Then

$$\bar{\partial} u = \frac{1}{4}\Big[\triangle f + \operatorname{div} \tilde{b} f + \tilde{b} \cdot \nabla f + i\Big(\frac{\partial(\tilde{b}_1 f)}{\partial y} - \frac{\partial(\tilde{b}_2 f)}{\partial x}\Big)\Big].$$

Plugging the above u into (3-6), we obtain

$$\int_{\mathcal{D}}\left[|\triangle f+\tilde{b}\cdot\nabla f|^2+|\operatorname{div}\tilde{b}f|^2+\left|\frac{\partial(\tilde{b}_1 f)}{\partial y}-\frac{\partial(\tilde{b}_2 f)}{\partial x}\right|^2\right]|P|^{-2}e^{\tau|z|^2} \geq C_3\tau\int_{\mathcal{D}}|\nabla f|^2|P|^{-2}e^{\tau|z|^2}-C_3\tau\int_{\mathcal{D}}|\tilde{b}|^2|f|^2|P|^{-2}e^{\tau|z|^2} + C_4\delta^{-2}\int_A|\nabla f|^2|P|^{-2}e^{\tau|z|^2}-C_4\delta^{-2}\int_A|\tilde{b}|^2|f|^2|P|^{-2}e^{\tau|z|^2}. \quad (3\text{-}7)$$

If we choose $u=f$ in (3-6), we get

$$\int_{\mathcal{D}}|\nabla f|^2|P|^{-2}e^{\tau|z|^2}\geq C_3\tau\int_{\mathcal{D}}|f|^2|P|^{-2}e^{\tau|z|^2}. \quad (3\text{-}8)$$

Since the norm of $\tilde{b}$ is chosen small enough, it is smaller than τ, which will be chosen large enough. With the aid of (3-8), we can incorporate the terms involving $\tilde{b}$ in the left-hand side of (3-7) into the first term in the right-hand side of (3-7):

$$\int_{\mathcal{D}}|\triangle f+\tilde{b}\cdot\nabla f|^2|P|^{-2}e^{\tau|z|^2} \geq C_5\tau\int_{\mathcal{D}}|\nabla f|^2|P|^{-2}e^{\tau|z|^2}+C_4\delta^{-2}\int_A|\nabla f|^2|P|^{-2}e^{\tau|z|^2}-C_4\delta^{-2}\int_A|\tilde{b}|^2|f|^2|P|^{-2}e^{\tau|z|^2}. \quad (3\text{-}9)$$

Furthermore, if $u=f$, the inequality (3-6) implies that

$$\int_{\mathcal{D}}|\nabla f|^2|P|^{-2}e^{\tau|z|^2}\geq C_4\delta^{-2}\int_A|f|^2|P|^{-2}e^{\tau|z|^2}. \quad (3\text{-}10)$$

Applying (3-10) to the last term in the right-hand side of (3-9) gives that

$$\int_{\mathcal{D}}|\triangle f+\tilde{b}\cdot\nabla f|^2|P|^{-2}e^{\tau|z|^2}\geq C_6\tau^2\int_{\mathcal{D}}|f|^2|P|^{-2}e^{\tau|z|^2}+C_7\delta^{-2}\int_A|\nabla f|^2|P|^{-2}e^{\tau|z|^2}. \quad (3\text{-}11)$$

We continue to get a refined estimate for the last term of (3-11). In order to achieve this goal, we need the following hypotheses for the geometry of the disk D_l and the parameter $\tau>1$:

(R1) The radius δ of each disk D_l is less than $a_4\tau^{-1}$.

(R2) The distance between any two distinct z_l is at least $2a_5\tau^{1/2}\delta$.

(R3) The total number of disks D_l is at most $a_6\tau$.

Under the those assumptions, we have these comparison estimates from [Donnelly and Fefferman 1990a]:

Lemma 8. *If $\bar{z}_1$ and $\bar{z}_2$ are any points in the same component A_l of A, then*:

(i) $a_7<e^{\tau|\bar{z}_1|^2}/e^{\tau|\bar{z}_2|^2}<a_8$.

(ii) $a_9<|P(\bar{z}_1)|/|P(\bar{z}_2)|<a_{10}$.

We also need the following Poincaré-type inequality on each annulus: if $f \in C^{\infty}(A_l)$ and f vanishes on the inner boundary of A_l, then

$$\int_{A_l} |\nabla f|^2 \geq a_{11}\delta^{-2} \int_{A_l} |f|^2. \tag{3-12}$$

The proof of (3-12) can be found in [Donnelly and Fefferman 1990a]. Let $z_l \in A_l$ be chosen arbitrarily. By Lemma 8, it follows that

$$\int_{A_l} |\nabla f|^2 |P(z)|^{-2} e^{\tau|z|^2} \geq C_8 \sum_l e^{\tau|z_l|^2} |P(z_l)|^{-2} \int_{A_l} |\nabla f|^2.$$

Since $f \in C_0^{\infty}\big(\mathbb{R}^2 \setminus \bigcup_l D_l(a)\big)$, the inequality (3-12) yields that

$$\int_{A_l} |\nabla f|^2 |P(z)|^{-2} e^{\tau|z|^2} \geq C_9 \sum_l e^{\tau|z_l|^2} |P(z_l)|^{-2} \delta^{-2} \int_{A_l} |f|^2.$$

Using Lemma 8 again, we obtain

$$\int_{A_l} |\nabla f|^2 |P(z)|^{-2} e^{\tau|z|^2} \geq C_{10}\delta^{-2} \int_{A} |f|^2 |P(z)|^{-2} e^{\tau|z|^2}.$$

Substituting the last inequality into the last term in (3-11) leads to

$$\int_{\mathfrak{D}} |\triangle f + \tilde{b}\cdot\nabla f|^2 |P|^{-2} e^{\tau|z|^2} \geq C_6\tau^2 \int_{\mathfrak{D}} |f|^2 |P|^{-2} e^{\tau|z|^2} + C_{11}\delta^{-4} \int_{A} |f|^2 |P|^{-2} e^{\tau|z|^2}. \tag{3-13}$$

We summarize the above arguments in the following proposition:

Proposition 9. *Assume* $f \in C_0^{\infty}\big(\mathbb{R}^2 \setminus \bigcup_l D_l(a)\big)$. *Then*:

(i) *It holds that*

$$\int_{\mathfrak{D}} |\triangle f + \tilde{b}\cdot\nabla f|^2 |P|^{-2} e^{\tau|z|^2} \geq C\tau^2 \int_{\mathfrak{D}} |f|^2 |P|^{-2} e^{\tau|z|^2}. \tag{3-14}$$

(ii) *If the additional assumptions* (R1)–(R3) *for* D_l *hold*, *the stronger inequality* (3-13) *is satisfied.*

4. Measure of singular sets

Let $\mathcal{M}$ be a compact smooth surface. In Section 2, we have shown that the Steklov eigenfunction e_λ vanishes at all points to order at most $C\lambda$. By the implicit function theorem, outside the singular sets, the nodal set is locally a 1-dimensional C^1 manifold. Adapting the arguments in [Donnelly and Fefferman 1990a] for (3-2), we can estimate those singular points in a quantitative way. We are able to obtain an upper bound for the singular points in terms of the eigenvalue λ.

Lemma 10. *Singular sets consist of at most finitely many points.*

Proof. Without loss of generality, we assume that $0 \in \mathcal{S}_\lambda$ and choose normal coordinates (x, y) at the origin. Next we prove there are finitely many singular points in $\bar{\mathcal{M}}$. Using Taylor expansion, we expand v locally at the origin. Then $v(x, y) = F_j(x, y) + W_{j+1}(x, y)$, where $F_j(x, y)$ consists of the leading nonvanishing term with homogenous order $j \geq 2$ and $W_{j+1}(x, y)$ is a higher-order reminder term. Since

$\triangle v+\bar{b}(z)\cdot\nabla v+\bar{q}(z)v=0$ and the coordinate is normal, we obtain that $\triangle F_j=0$. Under polar coordinates, we find that $F_j=r^j(a_1\cos(j\theta)+a_2\sin(j\theta))$. Obviously, $r^{-1}\,\partial F_j/\partial\theta$ and $\partial F_j/\partial r$ have no common zero if $r\neq 0$. Since

$$|\nabla F_j|^2=\left|\frac{\partial F_j}{\partial r}\right|^2+\frac{1}{r^2}\left|\frac{\partial F_j}{\partial\theta}\right|^2,$$

there exists a small neighborhood $\mathcal{U}$ of the origin such that $\mathcal{U}\cap\mathcal{S}_\lambda=0$. Since $\bar{\mathcal{M}}$ is compact, the lemma follows. □

We plan to count the number of singular points in a sufficiently small ball. Let $p\in\bar{\mathcal{M}}$. Consider a geodesic ball $\mathbb{B}(p, c\lambda^{-1/2})$. If c is small enough, then this geodesic ball is contained in a conformal chart. If we choose

$$w(z)=v(c\lambda^{-1/2}z)$$

with c sufficiently small then, from (3-1), w satisfies

$$\triangle w+\hat{b}(x)\cdot\nabla w+\hat{q}(x)w=0\quad\text{in }\mathbb{B}(0,4),\tag{4-1}$$

with $\hat{b}(x)=c\lambda^{-1/2}\bar{b}(x)$ and $\hat{q}(x)=c^2\lambda^{-1}\bar{q}(x)$. From (2-5), we obtain

$$\begin{cases}\|\hat{b}\|_{W^{1,\infty}(\mathbb{B}(0,4))}\le c\lambda^{1/2},\\ \|\hat{q}\|_{W^{1,\infty}(\mathbb{B}(0,4))}\le c^2\lambda,\end{cases}\tag{4-2}$$

with c sufficiently small.

Next we will count the total order of the vanishing of singular points for w in the sufficiently small ball. We study w in (4-1).

Proposition 11. *Suppose $z_l\in\mathcal{S}_\lambda\cap\mathbb{B}(p, c\lambda^{-1/2})$, where v vanishes to order n_l+1. Then $\sum_l n_l\le C\lambda$.*

Proof. It suffices to count the number of singular points of w in a small Euclidean ball with radius $\frac{1}{10}$ centered at the origin. Suppose that w vanishes to order n_l+1. Let $n_l=m_l+1$. We first consider the case $n_l\ge 2$. Then $m_l\ge 1$. Define the polynomial

$$P(z)=\prod(z-z_l)^{m_l}$$

with $|z_l|<\frac{1}{10}$. Let $\mathcal{D}=\mathbb{B}(0,2)$ and let D_l be small disjoint disks of radius δ centered at z_l. If $f\in C_0^\infty\big(\mathbb{R}^2\backslash\bigcup_l D_l\big)$, the inequality (3-14) in Proposition 9 implies that

$$\int_{\mathcal{D}}(|\triangle f|^2+|\hat{b}\cdot\nabla f|^2)|P|^{-2}e^{d_1\lambda|z|^2}\ge C_2\lambda^2\int_{\mathcal{D}}|f|^2|P|^{-2}e^{d_1\lambda|z|^2},\tag{4-3}$$

where $\tau=d_1\lambda$. We choose a cut-off function $\theta(z)$ such that θw has compact support in $\mathcal{D}$. We select the cut-off function $\theta\in C_0^\infty\big(\mathcal{D}\backslash\bigcup_l D_l\big)$ with the following properties:

(i) $\theta(z)=1$ if $|z|<\frac{3}{2}$ and $|z-z_l|>2\delta$.

(ii) $|\nabla\theta|<C_3$ and $|\triangle\theta|<C_4$ if $|z|>\frac{3}{2}$.

(iii) $|\nabla\theta|<C_5\delta^{-1}$ and $|\triangle\theta|<C_6\delta^{-2}$ if $|z-z_l|<2\delta$.

Substituting $f=\theta w$ into (4-3) yields that

$$\int_{(|z|<3/2)\cup(3/2\le|z|\le 2)} |\triangle(\theta w)+\tilde{b}\cdot\nabla(\theta w)|^2|P|^{-2}e^{d_1\lambda|z|^2} \ge C_2\lambda^2\int_{|z|<3/2}|w|^2|P|^{-2}e^{d_1\lambda|z|^2}.$$

From (4-1),

$$\triangle(\theta w)+\hat{b}\cdot\nabla(\theta w)=-\hat{q}\theta w+\triangle\theta w+2\nabla\theta\cdot\nabla w+\hat{b}\cdot\nabla\theta w.$$

By the assumption on θ, we obtain

$$|\triangle\theta w|+|\nabla\theta\cdot\nabla w|+|\nabla\theta w|\le C_7\delta^{m_l} \quad \text{if } |z-z_l|\le 2\delta.$$

Taking $\delta\to 0$, by the dominated convergence theorem, we have

$$c\lambda^2\int_{|z|<3/2}|w|^2|P|^{-2}e^{d_1\lambda|z|^2}+C_9(1+\lambda)^2\int_{3/2\le|z|\le 2}(|w|^2+|\nabla w|^2)|P|^{-2}e^{d_1\lambda|z|^2} \ge C_{10}\lambda^2\int_{|z|<3/2}|w|^2|P|^{-2}e^{d_1\lambda|z|^2}. \quad (4\text{-}4)$$

Since c is sufficiently small, we can absorb the first term in the left-hand side of (4-4) into the right-hand side. Then

$$\int_{3/2\le|z|\le 2}(|w|^2+|\nabla w|^2)|P|^{-2}e^{d_1\lambda|z|^2}\ge C_{11}\int_{|z|\le 1/2}|w|^2|P|^{-2}e^{d_1\lambda|z|^2}. \quad (4\text{-}5)$$

Obviously, it follows that

$$\max_{|z|\ge 3/2}|P|^{-2}\int_{3/2\le|z|\le 2}(|w|^2+|\nabla w|^2)e^{d_1\lambda|z|^2}\ge C_{11}\big(\min_{|z|\le 1/2}|P|^{-2}\big)\int_{|z|\le 1/2}|w|^2. \quad (4\text{-}6)$$

By standard elliptic theory, the last inequality implies

$$\max_{|z|\ge 3/2}|P|^{-2}e^{d_2\lambda}\int_{|z|\le 5/2}|w|^2\ge C_{11}\big(\min_{|z|\le 1/2}|P|^{-2}\big)\int_{|z|\le 1/2}|w|^2. \quad (4\text{-}7)$$

We claim that

$$e^{d_3\sum m_l}\le\frac{\min_{|z|\le 1/2}|P|^{-2}}{\max_{|z|\ge 3/2}|P|^{-2}}. \quad (4\text{-}8)$$

To prove (4-8), it suffices to verify

$$e^{-d_4\sum m_l}\min_{|z|\ge 3/2}|P|\ge\max_{|z|\le 1/2}|P| \quad (4\text{-}9)$$

away from the singular point z_l. Clearly,

$$\max_{|z|\le 1/2}|P|\le\big(\tfrac{1}{2}\big)^{\sum m_l}.$$

Since $z_l\in\mathbb{B}\big(0,\frac{1}{10}\big)$, we have

$$\big(\tfrac{3}{4}\big)^{\sum m_l}\le\min_{|z|\ge 3/2}|P|.$$

Combining the last two inequalities, we obtain (4-9). The claim is shown. Let's return to (4-7); we get

$$\frac{\min_{|z|\le 1/2}|P|^{-2}}{\max_{|z|\ge 3/2}|P|^{-2}} \le \frac{e^{d_5\lambda}\int_{|z|\le 5/2}|w|^2}{C_{11}\int_{|z|\le 1/2}|w|^2} \le e^{d_6\lambda}, \tag{4-10}$$

where we applied doubling estimates in the last inequality. Thanks to (4-8), we obtain

$$\sum m_l \le d_7\lambda.$$

Since $n_l = m_l + 1 \le 2m_l$, we complete the lemma for $n_l \ge 2$.

If the vanishing order for the singular point is two, i.e., $n_l = 1$. We consider $Q(z) = \prod (z - z_l)^{n_l/2}$ instead of $P(z)$. In this case, $Q(z)$ may not be defined as a single-valued holomorphic function on $\mathscr{C}$. We pass to a finite-branched cover of the disk $\mathfrak{D}$ punctured at z_l. The Carleman estimates in the previous sections still work. The same conclusion will follow. □

Based on the vanishing order estimate in Proposition 11, we are able to count the number of singular points.

Proof of Theorem 2. We cover the double manifold $\bar{\mathcal{M}}$ by geodesic balls with radius $C\lambda^{-1/2}$. Since $\bar{\mathcal{M}}$ is compact, the order of those balls is $C\lambda$. From Proposition 11, the conclusion in Theorem 2 follows. □

Remark 12. Thanks to Proposition 11, we can actually show a stronger result. Let $z_l \in \mathcal{M}$ be a singular point with vanishing order $n_l + 1$. Then $\sum_l n_l \le C\lambda^2$.

5. Growth of eigenfunctions

In this section, we will show that the eigenfunctions do not grow rapidly on too many small balls. We still restrict v to the small geodesic ball $\mathbb{B}(p, c\lambda^{-1/2})$ in the conformal chart. Let $w(z) = v(c\lambda^{-1/2}z)$. Then w satisfies the elliptic equation (4-1) with assumptions (4-2) in a Euclidean ball of radius 4 centered at the origin. If we suppose that w grows rapidly, that is,

$$C_1\int_{(1-3a)\delta\le|z-z_l|\le(1-3a/4)\delta} w^2 \le \int_{(1-3a/2)\delta\le|z-z_l|\le(1-a)\delta} w^2 \tag{5-1}$$

for all l and some large C_1, then the following proposition is valid:

Proposition 13. *Suppose D_l are disks contained in a Euclidean ball of radius $\frac{1}{30}$ centered at the origin. Furthermore, assume that*

(R1) $\delta < d_1\lambda^{-1}$, *and*

(R2) $|z_l - z_k| > d_2\lambda^{1/2}\delta$ *when* $l \ne k$.

If (5-1) *holds for all l, the number of disks D_l is less than $d_3\lambda$.*

Proof. We will use the stronger Carleman estimates in (3-13) in Proposition 9. We prove it by contradiction. Suppose that the collection $D_l = \{z \mid |z - z_l| \le \delta\}$ are disjoint disks satisfying the hypotheses (R1)–(R3) in Section 3. Without loss of generality, we require that all the D_l are in a ball centered at the origin with radius $\frac{1}{30}$. As before, $D_l(a) = \{z \mid |z - z_l| \le (1 - 2a)\delta\}$, where a is a suitably small positive constant. Let

$\mathcal{D}$ be a ball centered at the origin with radius 2. We choose a cut-off function $\theta \in C_0^\infty\big(\mathcal{D}\setminus \bigcup_l D_l\big)$ and assume $\theta(z)$ satisfies the following properties:

(i) $\theta(z) = 1$ if $|z| < 1$ and $|z - z_l| > \big(1 - \frac{3}{2}a\big)\delta$ for all l.

(ii) $|\nabla\theta| + |\triangle\theta| < C_2$ if $|z| > 1$.

(iii) $|\nabla\theta| < C_3\delta^{-1}$ and $|\triangle\theta| < C_4\delta^{-2}$ if $|z - z_l| < \big(1 - \frac{3}{2}a\big)\delta$.

Substituting $f = \theta w$ into (3-13) gives that

$$\int_{\mathcal{D}} |\triangle(\theta w)+\hat{b}\cdot\nabla(\theta w)|^2|P|^{-2}e^{d_4\lambda|z|^2} \ge C_5\lambda^2\int_{\mathcal{D}}|\theta w|^2|P|^{-2}e^{d_4\lambda|z|^2}+C_6\delta^{-4}\int_A|\theta w|^2|P|^{-2}e^{d_4\lambda|z|^2}. \quad (5\text{-}2)$$

We also assume $\tau = d_4\lambda$. Recall that $A = \bigcup_l A_l$ and $A_l = \{z \mid (1-2a)\delta \le |z - z_l| \le (1-a)\delta\}$. We first consider the integral in the left-hand side of the last inequality. Again, by (4-1),

$$\triangle(\theta w) + \hat{b}\cdot\nabla(\theta w) = -\hat{q}\theta w + \triangle\theta w + 2\nabla\theta\cdot\nabla w + \hat{b}\cdot\nabla\theta w.$$

Thus,

$$|\triangle(\theta w) + \hat{b}\cdot\nabla(\theta w)|^2 \le C(c\lambda^2\theta^2 w^2 + |\triangle\theta|^2 w^2 + |\nabla\theta|^2|\nabla w|^2 + c\lambda|\nabla\theta|^2 w^2),$$

where c is sufficiently small. We will absorb the term involving $\theta^2 w^2$ into the right-hand side of (5-2). Since c is small enough, we get

$$\int_{\mathcal{D}}(|\triangle\theta|^2 w^2 + c|\nabla\theta|^2 w^2 + |\nabla\theta|^2|\nabla w|^2)|P|^{-2}e^{d_4\lambda|z|^2} \ge C_7\lambda^2\int_{\mathcal{D}}|\theta w|^2|P|^{-2}e^{d_4\lambda|z|^2} + C_8\delta^{-4}\int_A|\theta w|^2|P|^{-2}e^{d_4\lambda|z|^2}. \quad (5\text{-}3)$$

Using the properties of $\theta(z)$ and taking into account that each D_l lies in the ball centered at the origin with radius $\frac{1}{30}$, we obtain

$$\int_{\mathcal{D}}(|\triangle\theta|^2 w^2 + c|\nabla\theta|^2 w^2 + |\nabla\theta|^2|\nabla w|^2)|P|^{-2}e^{d_4\lambda|z|^2} \ge C_7\lambda^2\int_{1/4\le|z|\le 1/2}|w|^2|P|^{-2}e^{d_4\lambda|z|^2} + C_9\delta^{-4}\sum_l\int_{(1-3a/2)\delta\le|z-z_l|\le(1-a)\delta}|w|^2|P|^{-2}e^{d_4\lambda|z|^2}. \quad (5\text{-}4)$$

Next we want to control the left-hand side of the last inequality. Write

$$\int_{\mathcal{D}}(|\triangle\theta|^2 w^2 + c|\nabla\theta|^2 w^2 + |\nabla\theta|^2|\nabla w|^2)|P|^{-2}e^{d_4\lambda|z|^2} = I + \sum_l I_l, \quad (5\text{-}5)$$

where

$$I = \int_{1\le|z|\le 2}(|\triangle\theta|^2 w^2 + c|\nabla\theta|^2 w^2 + |\nabla\theta|^2|\nabla w|^2)|P|^{-2}e^{d_4\lambda|z|^2},$$

$$I_l = \int_{(1-2a)\delta\le|z-z_l|\le(1-3a/2)\delta}(|\triangle\theta|^2 w^2 + c|\nabla\theta|^2 w^2 + |\nabla\theta|^2|\nabla w|^2)|P|^{-2}e^{d_4\lambda|z|^2}.$$

By standard elliptic estimates,

$$I \le e^{d_5\lambda} \max_{|z|\ge 1} |P|^{-2} \int_{3/4\le|z|\le 5/2} w^2. \tag{5-6}$$

Similarly, via elliptic estimates,

$$I_l \le C_{10}\delta^{-4}\big(\max_{A_l} |P|^{-2} e^{d_4\lambda|z|}\big) \int_{(1-3a)\delta\le|z-z_l|\le(1-3a/4)\delta} w^2. \tag{5-7}$$

Thanks to Lemma 8,

$$I_l \le C_{11}\delta^{-4}\big(\min_{A_l} |P|^{-2} e^{d_4\lambda|z|}\big) \int_{(1-3a)\delta\le|z-z_l|\le(1-3a/4)\delta} w^2. \tag{5-8}$$

Combining these inequalities together in (5-4) leads to

$$e^{d_5\lambda} \max_{|z|\ge 1} |P|^{-2} \int_{3/4\le|z|\le 5/2} w^2 + C_{11}\delta^{-4} \sum_l \big(\min_{A_l} |P|^{-2} e^{d_4\lambda|z|}\big) \int_{(1-3a)\delta\le|z-z_l|\le(1-3a/4)\delta} w^2$$
$$\ge C_{12} \min_{|z|\le 1/2} |P|^{-2} \int_{1/4\le|z|\le 1/2} |w|^2 + C_{13}\delta^{-4} \sum_l \min_{A_l}(|P|^{-2} e^{d_4\lambda|z|^2}) \int_{(1-3a/2)\delta\le|z-z_l|\le(1-a)\delta} w^2. \tag{5-9}$$

Performing similar arguments as for (4-8) shows that

$$\min_{|z|\le 1/2} |P|^{-2} > \max_{|z|\ge 1} |P|^{-2} e^{d_5 \sum_l m_l}.$$

If the number of the D_l is $d_3\lambda$, then

$$\min_{|z|\le 1/2} |P|^{-2} > \max_{|z|\ge 1} |P|^{-2} e^{d_6\lambda}. \tag{5-10}$$

We claim that

$$e^{C_{14}\lambda} \int_{1/4\le|z|\le 1/2} w^2 \ge \int_{3/4\le|z|\le 5/2} w^2. \tag{5-11}$$

We prove the claim by doubling estimates shown in Proposition 5. We choose a ball $\mathbb{B}\big(x_0, \frac{1}{8}\big) \subset \big\{z \;\big|\; \frac{1}{4} \le |z| \le \frac{1}{2}\big\}$. It is clear that

$$\int_{1/4\le|z|\le 1/2} w^2 \ge \int_{\mathbb{B}(x_0,1/8)} w^2.$$

Using doubling estimates, we have

$$e^{C_{15}\lambda} \int_{\mathbb{B}(x_0,1/8)} w^2 \ge \int_{\mathbb{B}(x_0,2/8)} w^2.$$

By finite iterations, we can find a large ball $\mathbb{B}(x_0, 3)$ that contains $\big\{z \;\big|\; \frac{3}{4} \le |z| \le \frac{5}{2}\big\}$. This yields that

$$\int_{\mathbb{B}(x_0,3)} w^2 \ge \int_{3/4\le|z|\le 5/2} w^2.$$

Then the combination of these inequalities verifies the claim.

If we choose d_3 suitably large, since the number of disks D_l is $d_3\lambda$, also d_6 is suitably large. From the inequalities (5-10) and (5-11), it follows that

$$e^{d_5\lambda}\max_{|z|\ge 1}|P|^{-2}\int_{3/4\le|z|\le 5/2} w^2 < C_{12}\min_{|z|\le 1/2}|P|^{-2}\int_{1/4\le|z|\le 1/2} w^2. \tag{5-12}$$

This contradicts the estimates (5-1) and (5-9). The proposition is proved. □

6. Growth estimates and nodal length

The purpose of this section is to find the connection between growth of eigenfunctions and nodal length. A suitable small growth in L^2 norm implies an upper bound on nodal length. We consider the second-order elliptic equations

$$\triangle\overline{w}+b^*\cdot\nabla\overline{w}+q^*\overline{w}=0 \quad \text{in } \mathbb{B}(0,4). \tag{6-1}$$

Assume that there exists a positive constant C such that $\|b^*\|_{W^{1,\infty}}\le C$ and $\|q^*\|_{W^{1,\infty}}\le C$. The following lemma relies on the Carleman estimates in Lemma 4. Suppose ϵ_1 is a sufficiently small positive constant.

Lemma 14. *Suppose that w satisfies the growth estimate*

$$\int_{(1-3a/2)\epsilon_0<r<(1-a)\epsilon_0}\overline{w}^2\le C_3\int_{(1-3a)\epsilon_0<r<(1-4a/3)\epsilon_0}\overline{w}^2, \tag{6-2}$$

where a and ϵ_0 are fixed small constants. Then, for $0<\epsilon_1<\frac{1}{100}\epsilon_0$, we have

$$\max_{r\le\epsilon_1}|\overline{w}|\ge C_4\left(\frac{\epsilon_1}{\epsilon_0}\right)^{C_5}\left(⨍_{\mathbb{B}(0,(1-4/3a)\epsilon_0)}\overline{w}^2\right)^{\frac12}, \tag{6-3}$$

where $⨍$ denotes the average of the integration.

Proof. We select a radial cut-off function $\theta\in C_0^\infty\big(\frac12\epsilon_1<r<\big(1-\frac{11}{10}a\big)\epsilon_0\big)$ that satisfies the properties:

(i) $\theta(r)=1$ for $\frac34\epsilon_1<r<\big(1-\frac{10}{9}a\big)\epsilon_0$.

(ii) $|\nabla\theta|+|\triangle\theta|\le C_6$ for $r>\big(1-\frac{10}{9}a\big)\epsilon_0$.

(iii) $|\nabla\theta|\le C_7\epsilon_1^{-1}$ and $|\triangle\theta|<C_8\epsilon_1^{-2}$ for $r\le\frac34\epsilon_1$.

From (6-1), we get

$$\triangle(\theta\overline{w})+b^*\cdot\nabla(\theta\overline{w})+q^*\theta\overline{w}=\triangle\theta\,\overline{w}+2\nabla\theta\cdot\nabla\overline{w}+b^*\cdot\nabla\theta\,\overline{w}.$$

Assume that $\tau>C$ is large enough. Substituting $u=\theta\overline{w}$ in Lemma 4 yields that

$$C_2\tau^3\int r^{\epsilon}e^{2\tau\phi(r)}\theta^2\overline{w}^2\,dr\,d\omega\le I, \tag{6-4}$$

where

$$I=\int r^4e^{2\tau\phi(r)}|\triangle\theta\,\overline{w}+2\nabla\theta\cdot\nabla\overline{w}+b^*\cdot\nabla\theta\,\overline{w}|^2\,dr\,d\omega.$$

Note that $\phi(r)$ is a decreasing function. Furthermore, by the assumptions on $\theta(z)$, we obtain

$$I \le e^{2\tau\phi(\epsilon_1/2)} \int_{\epsilon_1/2<r<3\epsilon_1/4} |\triangle\theta\overline{w} + 2\nabla\theta\cdot\nabla\overline{w} + b^*\cdot\nabla\theta\overline{w}|^2 r\,dr\,d\omega \\ + e^{2\tau\phi((1-10a/9)\epsilon_0)} \int_{(1-10a/9)\epsilon_0<r<(1-11a/10)\epsilon_0} |\triangle\theta\overline{w} + 2\nabla\theta\cdot\nabla\overline{w} + b^*\cdot\nabla\theta\overline{w}|^2 r\,dr\,d\omega.$$

By standard elliptic estimates, we derive that

$$I \le C_9 e^{2\tau\phi(\epsilon_1/2)} \int_{\epsilon_1/4<r<\epsilon_1} \overline{w}^2 r\,dr\,d\omega + C_{10} e^{2\tau\phi((1-10a/9)\epsilon_0)} \int_{(1-3a/2)\epsilon_0<r<(1-a)\epsilon_0} \overline{w}^2 r\,dr\,d\omega. \tag{6-5}$$

Taking the inequality (6-4) and assumptions of θ into account, we have

$$C_{10} e^{2\tau\phi((1-10a/9)\epsilon_0)} \int_{(1-3a/2)\epsilon_0<r<(1-a)\epsilon_0} \overline{w}^2 r\,dr\,d\omega + C_9 e^{2\tau\phi(\epsilon_1/2)} \int_{\epsilon_1/4<r<\epsilon_1} \overline{w}^2 r\,dr\,d\omega \\ \ge C_2\tau^3 \int_{3\epsilon_1/4<r<(1-10a/9)\epsilon_0} r^{\epsilon} e^{2\tau\phi(r)} \overline{w}^2\,dr\,d\omega \\ \ge C_2\tau^3 \big((1-\tfrac{10}{9}a)\epsilon_0\big)^{\epsilon-1} \int_{3\epsilon_1/4<r<(1-10a/9)\epsilon_0} e^{2\tau\phi(r)} \overline{w}^2 r\,dr\,d\omega. \tag{6-6}$$

Since ϵ and ϵ_0 are fixed positive constants, taking τ large enough we obtain

$$\tfrac{1}{2} C_2\tau^3 \big((1-\tfrac{10}{9}a)\epsilon_0\big)^{\epsilon-1} > C_{10}.$$

Taking the hypothesis (6-2) into consideration, we can incorporate the first term in the left-hand side of (6-6) into the right-hand side. It follows that

$$C_9 e^{2\tau\phi(\epsilon_1/2)} \int_{\epsilon_1/4<r<\epsilon_1} \overline{w}^2 r\,dr\,d\omega \ge C_{10} e^{2\tau\phi((1-10a/9)\epsilon_0)} \int_{3\epsilon_1/4<r<(1-10a/9)\epsilon_0} \overline{w}^2 r\,dr\,d\omega. \tag{6-7}$$

Fix such a τ; adding the term

$$e^{2\tau\phi((1-10a/9)\epsilon_0)} \int_{r<3\epsilon_1/4} \overline{w}^2 r\,dr\,d\omega$$

to both sides of the last inequality yields that

$$e^{2\tau\phi(\epsilon_1/2)} \int_{r<\epsilon_1} \overline{w}^2 r\,dr\,d\omega \ge C_{11} e^{2\tau\phi((1-10a/9)\epsilon_0)} \int_{r<(1-4a/3)\epsilon_0} \overline{w}^2 r\,dr\,d\omega, \tag{6-8}$$

where we have used the fact that ϕ is decreasing. Straightforward calculations show that

$$e^{2\tau(\phi((1-10a/9)\epsilon_0)-\phi(\epsilon_1/2))} \ge C_{13}\Big(\frac{\epsilon_1}{\epsilon_0}\Big)^{C_{12}}.$$

Thus,

$$\int_{r<\epsilon_1} \overline{w}^2 r\,dr\,d\omega \ge C_{13}\Big(\frac{\epsilon_1}{\epsilon_0}\Big)^{C_{12}} \int_{r<(1-4a/3)\epsilon_0} \overline{w}^2 r\,dr\,d\omega. \tag{6-9}$$

This completes the lemma. □

Our next goal is to find the relation between Lemma 14 and nodal length. We assume that the estimate (6-2) exists. Then the conclusion (6-3) in Lemma 14 holds. For $\epsilon_1 \le \frac{1}{100}\epsilon$, if $|z| < \epsilon_1$ then using Taylor's expansion gives that

$$\left|\overline{w}(z) - \sum_{|\alpha|\le C_5} \frac{1}{\alpha!}\frac{\partial^\alpha \overline{w}}{\partial z^\alpha}(0) z^\alpha\right| \le \sup_{|z|\le\epsilon_1} \sup_{|\alpha|=C_5+1} d_1 \left|\frac{\partial^\alpha \overline{w}}{\partial z^\alpha}(z)\right| {\epsilon_1}^{C_5+1},$$

where $\alpha = (\alpha_1, \alpha_2)$ and $\partial/\partial z^\alpha = \partial/\partial {z_1}^{\alpha_1} \cdot \partial/\partial {z_2}^{\alpha_2}$. To control the right-hand side of the last inequality, by elliptic estimates and a rescaling argument we have

$$\left|\overline{w}(z) - \sum_{|\alpha|\le C_5} \frac{1}{\alpha!}\frac{\partial^\alpha \overline{w}}{\partial z^\alpha}(0) z^\alpha\right| \le d_2 \left(\fint_{\mathbb{B}(0,(1-4a/3)\epsilon_0)} \overline{w}^2 \right)^{\frac{1}{2}} \left(\frac{\epsilon_1}{\epsilon_0}\right)^{C_5+1}.$$

Using the estimate (6-3) in Lemma 14, we get

$$\left|\overline{w}(z) - \sum_{|\alpha|\le C_5} \frac{1}{\alpha!}\frac{\partial^\alpha \overline{w}}{\partial z^\alpha}(0) z^\alpha\right| \le d_3 \left(\frac{\epsilon_1}{\epsilon_0}\right) \max_{|z|\le\epsilon_1} |\overline{w}|.$$

Choosing ϵ_1/ϵ_0 sufficiently small, by the triangle inequality we obtain

$$\sup_{|\alpha|\le C_5} \left|\frac{\partial^\alpha \overline{w}}{\partial z^\alpha}(0)\right| {\epsilon_1}^{|\alpha|} \ge d_4 \max_{|z|\le\epsilon_1} |\overline{w}|.$$

Applying again the estimate (6-3) to the right-hand side of the last inequality yields that

$$\sup_{|\alpha|\le C_5} \left|\frac{\partial^\alpha \overline{w}}{\partial z^\alpha}(0)\right| {\epsilon_0}^{|\alpha|} \ge d_5 \left(\fint_{\mathbb{B}(0,(1-4a/3)\epsilon_0)} \overline{w}^2 \right)^{\frac{1}{2}}. \tag{6-10}$$

By standard elliptic estimates, we also have

$$\sup_{|z|\le\epsilon_0/2} \sup_{|\alpha|\le C_5+1} \left|\frac{\partial^\alpha \overline{w}}{\partial z^\alpha}(z)\right| {\epsilon_0}^{|\alpha|} \le d_6 \left(\fint_{\mathbb{B}(0,(1-4a/3)\epsilon_0)} \overline{w}^2 \right)^{\frac{1}{2}}. \tag{6-11}$$

The basic relationship between derivatives and nodal length in two dimensions is shown in [Donnelly and Fefferman 1990a].

Lemma 15. *Suppose that $\overline{w}$ satisfies* (6-10) *and* (6-11). *Then*

$$H^1\big(z \bigm| |z| \le d_7\bar{\epsilon} \text{ and } \overline{w}(z) = 0\big) \le d_8\bar{\epsilon}.$$

With the aid of the last lemma, we can readily obtain an upper nodal length estimate.

Proposition 16. *Let $\overline{w}$ be the solution of* (6-1). *Suppose that $\bar{\epsilon} \le \epsilon_0$ and w satisfies the growth condition*

$$\int_{(1-3a/2)\bar{\epsilon}<r<(1-a)\bar{\epsilon}} \overline{w}^2 \le C_3 \int_{(1-3a)\bar{\epsilon}<r<(1-4a/3)\bar{\epsilon}} \overline{w}^2. \tag{6-12}$$

Then

$$H^1\big(z \bigm| |z| \le d_9\bar{\epsilon} \text{ and } \overline{w}(z) = 0\big) \le d_{10}\bar{\epsilon}.$$

Proof. Since the inequalities (6-10) and (6-11) can be derived from (6-12) by Lemma 14, the proposition follows from the last lemma. □

7. Total nodal length

As Proposition 13 indicates, the eigenfunctions cannot grow rapidly on too many small balls. If they grow slowly, we have an upper bound on the local length of nodal sets by Proposition 16. In this section, we will link these two arguments together. To achieve it, we will employ a process of repeated subdivision and selection of squares. The idea is inspired by [Donnelly and Fefferman 1990a].

Assume that $\mathbb{B}(p, c\lambda^{-1/2})$ is a geodesic ball of the double manifold $\bar{\mathcal{M}}$. Choosing c to be small, it is contained in a conformal chart. Let $w(z) = v(c\lambda^{-1/2}z)$ with c sufficiently small. We know that w satisfies

$$\triangle w + \hat{b}(x) \cdot \nabla w + \hat{q}(x) w = 0 \quad \text{in } \mathbb{B}(0, 4). \tag{7-1}$$

We consider the square $P = \{(x, y) \mid \max(|x|, |y|) \le \frac{1}{60}\}$ in $\mathbb{B}(0, 4)$ and divide it into a grid of closed squares P_l with side $\delta \le a_1\lambda^{-1}$. If (5-1) holds for some point $z_l \in P_l$ and for some sufficiently large C_1, we call P_l a square of rapid growth. With the aid of Proposition 13, we are able to obtain the following result:

Lemma 17. *There are at most $C\lambda^2$ squares with side δ where w is of rapid growth.*

Proof. Let I_1 be the collection of those indices l for which P_l is a square of rapid growth. For each $l \in I_1$, there exists some point $z_l \in P_l$ such that (5-1) holds. Let $|I_1|$ denote the cardinality of I_1. Define

$$P_l^* = \{z \mid |z - z_l| < d_1\delta\lambda^{1/2}\}.$$

The collection of disks P_l^* covers the collection of squares P_l for $l \in I_1$. We choose a maximal collection of disjoint disks of P_l^* and denote it as I_2. If $l \in I_2$, we define

$$P_l^{**} = \{z \mid |z - z_l| < 4d_1\delta\lambda^{1/2}\}.$$

Since the collection of disks in I_2 is maximal and they are disjoint, we obtain that

$$\bigcup_{l\in I_2} P_l^{**} \supseteq \bigcup_{l\in I_1} P_l^{*} \supseteq \bigcup_{l\in I_1} P_l.$$

Thus,

$$|I_2| \times 16 d_1^2 \delta^2 \lambda \ge |I_1|\delta^2,$$

which implies

$$|I_2|\lambda \ge d_2|I_1|.$$

Recall from Proposition 13 that $|I_2| \le d_3\lambda$. Therefore, we obtain the desirable estimate $|I_1| \le d_4\lambda^2$. □

Now we introduce an iterative process of bisecting squares. We begin by dividing the square into a grid of squares $P_l(1)$ with side $\delta(1) = a_1\lambda^{-1}$, then separate them into two categories $R_l(1)$ and $S_l(1)$. $R_l(1)$ are those where w is of rapid growth and $S_l(1)$ are those where (5-1) fails for w. We continue to bisect each square $R_l(1)$ to obtain squares $P_l(2)$ with side $\delta(2) = \frac{1}{2}\delta(1)$. Again, we split $P_i(2)$ into the subcollection $R_l(2)$ with rapid growth and $S_l(2)$ with slow growth. We repeat the process at each step k. Then there are squares $R_l(k)$ and $S_l(k)$ with $\delta(k)=\frac{1}{2^k}\delta(1)$. We count the number of $R_l(k)$ and $S_l(k)$ at step k:

Lemma 18. (i) *The number of squares $R_l(k)$ is at most $C_2\lambda^2$.*

(ii) *The number of squares $S_l(k)$ is at most $C_3\lambda^2$.*

Proof. The conclusion (i) follows directly from Lemma 17. We only need to show (ii). If $k=1$, the conclusion (ii) follows because the total number of squares is at most of order λ^2. If $k\geq 2$ then, by construction of those squares,

$$|S_l(k)|\leq 4|R_l(k-1)|\leq C_4\lambda^2,$$

where we have used (i) in the last inequality. The lemma is done. □

The next lemma tells that almost every point lies in some $R_l(k)$ with slow growth. It is Lemma 6.3 in [Donnelly and Fefferman 1990a].

Lemma 19. $\bigcup_{k,l} S_l(k)$ *covers the square P except for singular points $\mathcal{S}=\{z\in P\mid w(x)=0,\ \nabla w=0\}$.*

We are ready to give the proof of Theorem 3.

Proof of Theorem 3. Consider $\overline{w}(z)=w(z_l+\epsilon_0^{-1}\delta(k)z)$. Then $\overline{w}(z)$ satisfies (6-1). Choosing a finite collection of $z_l\in S_l(k)$ and applying Proposition 16, we have

$$H^1\big(z\ \big|\ w(z)=0\ \text{ and }\ z\in S_l(k)\big)\leq C_5 2^{-k}\lambda^{-1}. \tag{7-2}$$

Furthermore, thanks to Lemma 19,

$$\begin{aligned} H^1\big(z\ \big|\ w(z)=0\ \text{ and }\ \max(|x|,|y|)\leq \tfrac{1}{60}\big) &\leq \sum_{l,k} H^1\big(z\ \big|\ w(z)=0\ \text{ and }\ z\in S_l(k)\big)\\ &\leq \lambda^2\sum_k C_5 2^{-k}\lambda^{-1}\leq C_6\lambda, \end{aligned} \tag{7-3}$$

where we have used (ii) in Lemma 18 and (7-2). Since $w(z)=v(c\lambda^{-1/2}z)$, by the rescaling argument, we obtain

$$H^1\big(\{v(z)=0\}\cap\mathbb{B}(p,c\lambda^{-1/2})\big)\leq C_6\lambda^{1/2}.$$

Finally, covering $\bar{\mathcal{M}}$ with order λ of geodesic balls with radius $c\lambda^{-1/2}$, we readily deduce that

$$H^1(z\in\bar{\mathcal{M}}\mid v(z)=0)\leq C_7\lambda^{3/2}.$$

Thus, so is $H^1(\mathcal{N}_\lambda)$. □

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References

[Bakri and Casteras 2014] L. Bakri and J.-B. Casteras, "Quantitative uniqueness for Schrödinger operator with regular potentials", *Math. Methods Appl. Sci.* **37**:13 (2014), 1992–2008. MR 3245115 Zbl 1301.35190

[Bellová and Lin 2015] K. Bellová and F.-H. Lin, "Nodal sets of Steklov eigenfunctions", *Calc. Var. Partial Differential Equations* **54**:2 (2015), 2239–2268. MR 3396451 Zbl 1327.35263

[Brüning 1978] J. Brüning, "Über Knoten von Eigenfunktionen des Laplace–Beltrami-Operators", *Math. Z.* **158**:1 (1978), 15–21. MR 0478247 Zbl 0349.58012

[Calderón 1980] A.-P. Calderón, "On an inverse boundary value problem", pp. 65–73 in *Seminar on numerical analysis and its applications to continuum physics* (Rio de Janeiro, 1980), Soc. Brasil. Mat., Rio de Janeiro, 1980. MR 590275

[Colding and Minicozzi 2011] T. H. Colding and W. P. Minicozzi, II, "Lower bounds for nodal sets of eigenfunctions", *Comm. Math. Phys.* **306**:3 (2011), 777–784. MR 2825508 Zbl 1238.58020

[Dong 1992] R.-T. Dong, "Nodal sets of eigenfunctions on Riemann surfaces", *J. Differential Geom.* **36**:2 (1992), 493–506. MR 1180391 Zbl 0776.53024

[Donnelly and Fefferman 1988] H. Donnelly and C. Fefferman, "Nodal sets of eigenfunctions on Riemannian manifolds", *Invent. Math.* **93**:1 (1988), 161–183. MR 943927 Zbl 0659.58047

[Donnelly and Fefferman 1990a] H. Donnelly and C. Fefferman, "Nodal sets for eigenfunctions of the Laplacian on surfaces", *J. Amer. Math. Soc.* **3**:2 (1990), 333–353. MR 1035413 Zbl 0702.58077

[Donnelly and Fefferman 1990b] H. Donnelly and C. Fefferman, "Nodal sets of eigenfunctions: Riemannian manifolds with boundary", pp. 251–262 in *Analysis, et cetera*, edited by P. H. Rabinowitz and E. Zehnder, Academic Press, Boston, 1990. MR 1039348 Zbl 0697.58055

[Girouard and Polterovich 2014] A. Girouard and I. Polterovich, "Spectral geometry of the Steklov problem", preprint, 2014. arXiv 1411.6567

[Han and Lin 2008] Q. Han and F.-H. Lin, "Nodal sets of solutions of elliptic differential equations", book in preparation, 2008, available at http://www.nd.edu/qhan/nodal.pdf.

[Hardt and Simon 1989] R. Hardt and L. Simon, "Nodal sets for solutions of elliptic equations", *J. Differential Geom.* **30**:2 (1989), 505–522. MR 1010169 Zbl 0692.35005

[Hezari and Sogge 2012] H. Hezari and C. D. Sogge, "A natural lower bound for the size of nodal sets", *Anal. PDE* **5**:5 (2012), 1133–1137. MR 3022851 Zbl 1329.35224

[Jost 1984] J. Jost, *Harmonic maps between surfaces*, Lecture Notes in Mathematics **1062**, Springer, Berlin, 1984. MR 754769 Zbl 0542.58002

[Lin 1991] F.-H. Lin, "Nodal sets of solutions of elliptic and parabolic equations", *Comm. Pure Appl. Math.* **44**:3 (1991), 287–308. MR 1090434 Zbl 0734.58045

[Polterovich et al. 2015] I. Polterovich, D. A. Sher, and J. A. Toth, "Nodal length of Steklov eigenfunctions on real-analytic Riemannian surfaces", preprint, 2015. arXiv 1506.07600

[Sogge and Zelditch 2011] C. D. Sogge and S. Zelditch, "Lower bounds on the Hausdorff measure of nodal sets", *Math. Res. Lett.* **18**:1 (2011), 25–37. MR 2770580 Zbl 1242.58017

[Sogge and Zelditch 2012] C. D. Sogge and S. Zelditch, "Lower bounds on the Hausdorff measure of nodal sets, II", *Math. Res. Lett.* **19**:6 (2012), 1361–1364. MR 3091613 Zbl 1283.58020

[Sogge et al. 2015] C. D. Sogge, X. Wang, and J. Zhu, "Lower bounds for interior nodal sets of Steklov eigenfunctions", preprint, 2015. To appear in *Proc. Amer. Math. Soc.* arXiv 1503.01091

[Wang and Zhu 2015] X. Wang and J. Zhu, "A lower bound for the nodal sets of Steklov eigenfunctions", *Math. Res. Lett.* **22**:4 (2015), 1243–1253. MR 3391885

[Zelditch 2008] S. Zelditch, "Local and global analysis of eigenfunctions on Riemannian manifolds", pp. 545–658 in *Handbook of geometric analysis, I*, edited by L. Ji et al., Adv. Lect. Math. **7**, International Press, 2008. MR 2483375 Zbl 1176.58017

[Zelditch 2014] S. Zelditch, "Measure of nodal sets of analytic Steklov eigenfunctions", preprint, 2014. arXiv 1403.0647

[Zhu 2015] J. Zhu, "Doubling property and vanishing order of Steklov eigenfunctions", *Comm. Partial Differential Equations* **40**:8 (2015), 1498–1520. MR 3355501 Zbl 1323.47017

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SOME COUNTEREXAMPLES TO SOBOLEV REGULARITY FOR DEGENERATE MONGE–AMPÈRE EQUATIONS

CONNOR MOONEY

We construct a counterexample to $W^{2,1}$ regularity for convex solutions to

$$\det D^2 u \leq 1, \quad u|_{\partial\Omega} = \text{const.}$$

in two dimensions. We also prove a result on the propagation of singularities of the form $|x_2|/|\log x_2|$ in two dimensions. This generalizes a classical result of Alexandrov and is optimal by example.

1. Introduction

In this paper we investigate the $W^{2,1}$ regularity of convex Alexandrov solutions to degenerate Monge–Ampère equations of the form

$$\det D^2 u(x) = \rho(x) \leq 1 \quad \text{in } \Omega, \quad u|_{\partial\Omega} = \text{const.}, \tag{1}$$

where Ω is a bounded convex domain in $\mathbb{R}^n$.

In the case that ρ also has a strictly positive lower bound, $W^{2,1}$ estimates were first obtained by De Philippis and Figalli [2013]. They showed that $\Delta u \log^k(2 + \Delta u)$ is integrable for any k. It was subsequently shown in [De Philippis et al. 2013; Schmidt 2013] that $D^2 u$ is in fact $L^{1+\epsilon}$ for some ϵ depending on dimension and $\|1/\rho\|_{L^\infty(\Omega)}$. These estimates are optimal in light of two-dimensional examples due to Wang [1995] with the homogeneity

$$u(\lambda x_1, \lambda^\alpha x_2) = \lambda^{1+\alpha} u(x_1, x_2).$$

These estimates fail when ρ degenerates. In three and higher dimensions, it is not hard to construct solutions to (1) that have a Lipschitz singularity on part of a hyperplane, so the second derivatives concentrate (see Section 2). However, in two dimensions, a classical result of Alexandrov [1942] shows that Lipschitz singularities of convex solutions to $\det D^2 u \leq 1$ propagate to the boundary. Thus, in two dimensions, solutions to (1) are C^1 and $D^2 u$ has no jump part. However, this leaves open the possibility that $D^2 u$ has nonzero Cantor part.

The main result of this paper is the construction of a solution to (1) in two dimensions that is not $W^{2,1}$. This negatively answers an open problem stated in both [De Philippis and Figalli 2014] and [Figalli 2015], which was motivated by potential applications to the semigeostrophic equation. We also prove that, in two

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dimensions, singularities that are logarithmically slower than Lipschitz propagate. This result generalizes the theorem of Alexandrov and is optimal by example.

The $W^{2,1}$ estimates mentioned above have applications to the global existence of weak solutions to the semigeostrophic equation [Ambrosio et al. 2012; 2014]. In this context, the density ρ solves a continuity equation that preserves L^∞ bounds. This is the only regularity property of ρ that is globally preserved, due to nonlinear coupling between ρ and the velocity field. It is therefore useful to obtain estimates that depend on L^∞ bounds for ρ but not on its regularity.

To apply the results in [De Philippis and Figalli 2013; De Philippis et al. 2013] one must assume that ρ is supported in the whole space. However, in physically interesting cases, the initial density is compactly supported. It is thus natural to ask what one can show about solutions to (1). Our construction shows that, even in two dimensions, one must rely more on the specific structure of the semigeostrophic equation to obtain existence results for compactly supported initial data.

The idea of our construction is to start with a one-dimensional convex function of x_2 in the half-space $\{x_1 < 0\}$ whose second derivative has nontrivial Cantor part, and extend to a convex function on $\mathbb{R}^2$ which lifts from these values without generating too much Monge–Ampère measure. To accomplish this we start with a "building block" v_1 that agrees with $|x_2|$ in $\{|x_2| \geq (x_1)_+^\alpha\}$ for some $\alpha > 1$, and in the cusp $\{|x_2| < (x_1)_+^\alpha\}$ grows with the homogeneity

$$v_1(\lambda x_1, \lambda^\alpha x_2) = \lambda^\alpha v_1(x_1, x_2).$$

By superposing vertically translated rescalings of (a smoothed version of) v_1 in a self-similar way, we obtain our example.

Our main theorem is:

Theorem 1.1. *For all $n \geq 2$, there exist solutions to* (1) *that are not $W^{2,1}$.*

Remark 1.2. It is obvious that solutions to (1) in one dimension are $C^{1,1}$.

Remark 1.3. In our examples, the support of ρ is irregular. In particular, in the higher-dimensional examples, the support of ρ is a cusp revolved around an axis, and in the two-dimensional example, the support of ρ has a very irregular "fractal" geometry.

In, e.g., [Daskalopoulos and Savin 2009; Guan 1997] the authors obtain interesting regularity results when ρ degenerates in a specific way, motivated by applications to prescribed Gauss curvature.

Our second result concerns the behavior of solutions to (1) near a single line segment in $\mathbb{R}^2$. Since Lipschitz singularities propagate, D^2u cannot concentrate on a line segment. (In our two-dimensional counterexample to $W^{2,1}$ regularity, D^2u concentrates on a family of horizontal rays.) On the other hand, by modifying an example in [Wang 1995] one can construct, for any $\epsilon > 0$, a solution to (1) that grows like $|x_2|/|\log x_2|^{1+\epsilon}$, with second derivatives not in $L \log^{1+\epsilon} L$ (see Section 4).

It is natural to ask whether one can take $\epsilon \leq 0$. We show that this is not possible. Indeed, we construct a family of barriers that agree with $|x_2|/|\log x_2|$ away from arbitrarily thin cusps around the x_1-axis, where we can make the Monge–Ampère measure as large as we like. By sliding these barriers we prove that singularities of the form $|x_2|/|\log x_2|$ propagate. Our second theorem is:

Theorem 1.4. *Assume that u is convex on $\mathbb{R}^2$ and that $\det D^2u \le 1$. Then if $u(0)=0$ and $u \ge c|x_2|/|\log x_2|$ in a neighborhood of the origin for some $c > 0$, then u vanishes on the x_1-axis.*

Remark 1.5. Note that we assume the growth in a neighborhood of 0. For a Lipschitz singularity it is enough to assume the growth at a point, which automatically extends to a neighborhood by convexity. (See, e.g., [Figalli and Loeper 2009] for a short proof that Lipschitz singularities propagate.)

Remark 1.6. Theorem 1.4 shows that a solution to $\det D^2u \ge 1$ in two dimensions cannot separate from a tangent plane more slowly than $r^2e^{-1/r}$ in any fixed direction. This quantifies the classical result that such functions are strictly convex. The idea is that if not, then after subtracting a tangent plane we have $0 \le u \le C|x_1| + x_2^2e^{-1/|x_2|}$ near the origin. Taking the Legendre transform one obtains $u^* \ge c|x_2|/|\log x_2|$ near the origin. Applying Theorem 1.4 to u^* gives a contradiction of the strict convexity of u.

The paper is organized as follows. In Section 2 we construct simple examples of solutions to (1) in the case $n \ge 3$ which have a Lipschitz singularity on a hyperplane. In Section 3 we construct a solution to (1) in two dimensions whose second derivatives have nontrivial Cantor part. This proves Theorem 1.1. In Section 4 we first construct examples showing that Theorem 1.4 is optimal. We then construct barriers related to these examples. Finally, we use the barriers to prove Theorem 1.4.

2. The case $n \ge 3$

In this section we construct simple examples of solutions to (1) in three and higher dimensions that have a Lipschitz singularity on a hyperplane. Denote $x \in \mathbb{R}^n$ by (x', x_n) and let $r = |x'|$. More precisely:

Proposition 2.1. *In dimension $n \ge 3$, for any $\alpha \ge \frac{n}{n-2}$ there exists a solution to* (1) *that is a positive multiple of $|x_n|$ in $\{|x_n| \ge (r-1)_+^{\alpha}\}$.*

Proof. Let $h(r) = (r-1)_+$. We search for a convex function $u = u(r, x_n)$ in $\{|x_n| < h(r)^\alpha\}$, with $\alpha > 1$, that glues "nicely" across the boundary to $|x_n|$. To that end we look for a function with the homogeneity

$$u(1+\lambda t, \lambda^\alpha x_n) = \lambda^\alpha u(1+t, x_n),$$

so that $\partial_n u$ is invariant under the rescaling. Let

$$u(r, x_n) = \begin{cases} h(r)^\alpha + h(r)^{-\alpha}x_n^2, & |x_n| < h(r)^\alpha, \\ 2|x_n|, & |x_n| \ge h(r)^\alpha. \end{cases}$$

Then ∇u is continuous on $\partial\{|x_n| < h(r)^\alpha\} \setminus \{r = 1, x_n = 0\}$. Furthermore, $\partial u|_{\{r=1, x_n=0\}}$ is the line segment between $\pm 2e_n$, which has measure zero. Thus, in the Alexandrov sense, $\det D^2u$ can be computed piecewise. In the cylindrical coordinates (r, x_n) one easily computes

$$\det D^2u = \begin{cases} \dfrac{1}{r^{n-2}}\left(2\alpha^{n-1}(\alpha-1)h(r)^{\alpha(n-2)-n}\left(1-\left(\dfrac{x_n}{h(r)^\alpha}\right)^2\right)^{n-1}\right), & |x_n| < h(r)^\alpha, \\ 0, & |x_n| \ge h(r)^\alpha. \end{cases}$$

For $\alpha \ge \frac{n}{n-2}$ the right-hand side is locally bounded. □

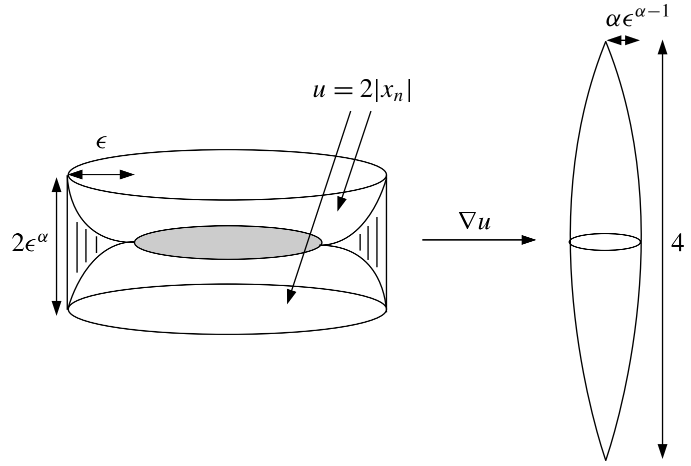

Figure 1. The gradient map of u decreases volume if $\alpha \geq \frac{n}{n-2}$.

Remark 2.2. The bound on α can be understood by looking at the gradient map of u, which takes a "ring" of volume like $h(r)^{1+\alpha}$ to a "football" with length of order 1 and radius of order $h(r)^{\alpha-1}$ (see Figure 1). Then impose that it decreases volume.

Remark 2.3. Observe that $\det D^2u$ grows like dist.$^{n-2-n/\alpha}$ from its zero set. This is in a sense optimal; if $\det D^2u < C|x_n|^{n-2}$ then one can modify Alexandrov's two-dimensional argument to show that the singularity has no extremal points.

3. The case $n = 2$

In this section we prove Theorem 1.1. We construct our example in several steps.

First, let $g(t)$ be a smooth, convex function such that $g(t) = \frac{1}{2}$ for $t \leq 0$ and $g(t) = t^\alpha$ for $t \geq 1$, where $\alpha > 1$. Then define

$$v_1(x_1, x_2) = \begin{cases} g(x_1) + \dfrac{1}{g(x_1)} x_2^2, & |x_2| < g(x_1), \\ 2|x_2|, & |x_2| \geq g(x_1). \end{cases}$$

It is easy to check that v_1 is a $C^{1,1}$ convex function, and in the Alexandrov sense,

$$\det D^2 v_1(x_1, x_2) = \begin{cases} 2\dfrac{g''(x_1)}{g(x_1)}\left(1 - \dfrac{x_2^2}{g(x_1)^2}\right), & |x_2| < g(x_1), \\ 0, & |x_2| \geq g(x_1). \end{cases}$$

In particular, $\det D^2 v_1$ is bounded, and decays like x_1^{-2} for x_1 large. Let v_λ be the rescalings defined by

$$v_\lambda(x_1, x_2) = \frac{1}{\lambda^{1+\alpha}} v_1(\lambda x_1, \lambda^\alpha x_2).$$

Observe that

$$\det D^2 v_\lambda(x_1, x_2) = \det D^2 v_1(\lambda x_1, \lambda^\alpha x_2),$$

and we have

$$v_\lambda = \frac{1}{\lambda}(x_1^\alpha + x_1^{-\alpha} x_2^2) \quad \text{in } \{x_1 \geq \lambda^{-1}\} \cap \{|x_2| \leq x_1^\alpha\}. \tag{2}$$

In the following key lemma we show that any superposition of λ vertical translated copies of v_λ has bounded Monge–Ampère measure in $\{x_1 > 1/2\}$, and separates from its tangent planes when we step away from the x_2-axis.

Lemma 3.1. *Let $\{x_{2,i}\}_{i=1}^N$ be fixed numbers with $|x_{2,i}| \leq 1$ for all i, where N is any positive integer. Let*

$$w(x_1, x_2) = \sum_{i=1}^N v_N(x_1, x_2 - x_{2,i}).$$

Then

$$\det D^2 w < C(\alpha) \quad \text{in } \left\{x_1 > \tfrac{1}{2}\right\} \tag{3}$$

for some $C(\alpha)$ independent of N and the choice of $\{x_{2,i}\}$, and

$$w(2, x_2) > w(0, x_2) + \mu(\alpha) \quad \text{for all } |x_2| < 1, \tag{4}$$

for some $\mu(\alpha) > 0$ independent of N and the choice of $\{x_{2,i}\}$.

Proof. We first prove (3). Since $\det D^2 v_1$ is bounded we may assume that $N \geq 2$. Consider a point $p = (p_1, p_2) \in \left\{x_1 > \tfrac{1}{2}\right\}$. Since w is $C^{1,1}$, the curves $p_2 = x_{2,i} \pm p_1^\alpha$ don't contribute anything to $\det D^2 w$, so we may assume that $p_2 \neq x_{2,i} \pm p_1^\alpha$ for any i. Then in a neighborhood of p, a subset of $M \leq N$ of the translates are not linear, and all are linear if in addition $|p_2| > 1 + p_1^\alpha$. Up to relabeling the indices and subtracting a linear function of x_2, by (2) we can write

$$w = \frac{M}{N}\left(x_1^\alpha + x_1^{-\alpha}\left(x_2^2 - 2x_2 \frac{1}{M}\sum_{i=1}^M x_{2,i} + \frac{1}{M}\sum_{i=1}^M x_{2,i}^2\right)\right)$$

in a neighborhood of p. Since $|x_{2,i}| \leq 1$, one easily computes that

$$\det D^2 w(p) \leq 2\alpha \frac{M^2}{N^2} p_1^{-2}\big(\alpha - 1 + (\alpha+1) p_1^{-2\alpha}(p_2^2 + 2|p_2| + 1)\big),$$

and $\det D^2 w(p) = 0$ if $|p_2| > 1 + p_1^\alpha$. We conclude that

$$\det D^2 w(p) < C(\alpha),$$

where $C(\alpha)$ does not depend on N.

To prove (4), since v_1 is monotone increasing in the e_1 direction, we have for $|x_2| \leq 2$ that

$$v_1(2, x_2) - v_1(0, x_2) \geq v_1(2, x_2) - v_1(2^{1/\alpha}, x_2) \geq 2^{-\alpha}(2^\alpha - 2)^2.$$

Since $\alpha > 1$, the lower bound $\mu := 2^{-\alpha}(2^\alpha - 2)^2$ is strictly positive.

By (2) the same argument gives

$$v_N(2, x_2) - v_N(0, x_2) > \frac{\mu}{N}$$

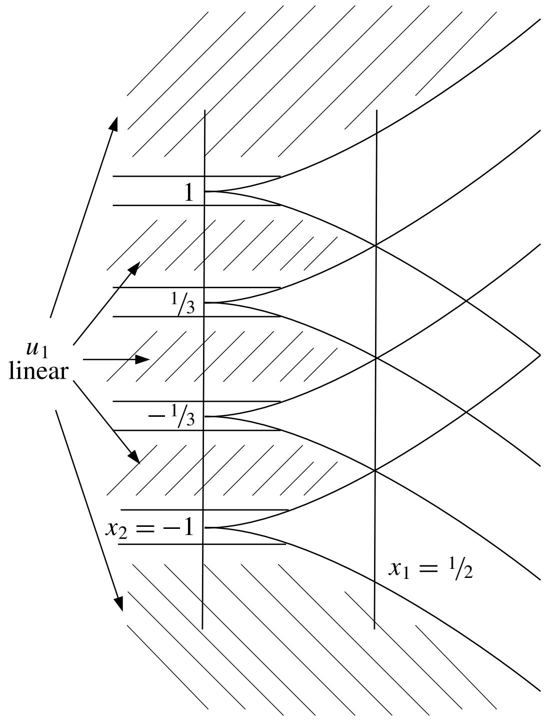

Figure 2. The function u_1 is a piecewise linear function of x_2 outside of the four equally spaced cusps between $x_2 = -1$ and $x_2 = 1$.

for $|x_2| \leq 2$. Finally, since $|x_{2,i}| \leq 1$, we have for $|x_2| < 1$ that

$$\sum_{i=1}^{N} \big(v_N(2, x_2 - x_{2,i}) - v_N(0, x_2 - x_{2,i}) \big) \geq \sum_{i=1}^{N} \frac{\mu}{N} = \mu > 0,$$

completing the proof □

We can now complete the construction. Roughly, at stage k we superpose 2^{k+1} vertical translations of $v_{2^{k+1}}$, starting at the endpoints of the intervals removed up to the k-th stage in the construction of the Cantor set.

Proof of Theorem 1.1. Fix

$$\alpha := \frac{\log 3}{\log 2},$$

and define

$$u_1(x_1, x_2) = \sum_{i=0}^{3} v_4(x_1, x_2 - 1 + 2i/3).$$

Then u_1 is a piecewise linear function of x_2 outside of four equally spaced cusps in $\{x_1 > 0\}$ connected to thin strips in $\{x_1 < 0\}$ (see Figure 2).

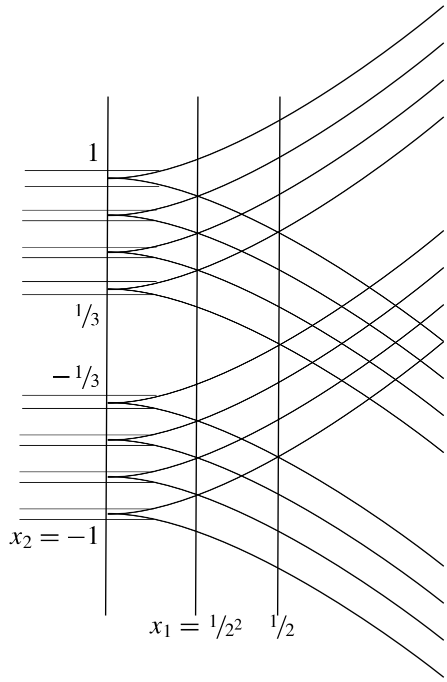

Figure 3. The function u_2 is obtained by superposing two rescaled copies of u_1, whose Hessians don't affect each other in $\{x_1 \le \frac{1}{2}\}$.

Define u_k inductively by

$$u_{k+1}(x_1, x_2) = \frac{1}{2^{1+\alpha}}\big(u_k\big(2x_1, 3\big(x_2 + \tfrac{2}{3}\big)\big) + u_k\big(2x_1, 3\big(x_2 - \tfrac{2}{3}\big)\big)\big).$$

We first claim that the $\det D^2 u_k$ are uniformly bounded (in k) in $\{x_1 > \frac{1}{2}\}$. Indeed, each u_k is a sum of 2^{k+1} vertical translates of $v_{2^{k+1}}$ by values in $[-1, 1]$, so this follows from (3).

Next we show that the $\det D^2 u_k$ are uniformly bounded in $\mathbb{R}^2$. Note that the u_k are linear functions of x_2 in $\{x_1 \le 1\} \times \{|x_2| > 2\}$, so in $\{x_1 \le \frac{1}{2}\}$, the rescaled copies of u_k in the definition of u_{k+1} are linear where the other is nontrivial (the determinants "don't interact"; see Figure 3). Since the rescaling $2^{-(1+\alpha)} u_k(2x_1, 3x_2)$ preserves Hessian determinants, we conclude that

$$\det D^2 u_{k+1}|_{\{x_1 \le 1/2\}} \le \sup_{x_1 \ge 0} \det D^2 u_k.$$

One easily checks that $\det D^2 u_1$ is bounded, so the claim follows by induction.

Since $|v_\lambda|, |\nabla v_\lambda| < C R^\alpha/\lambda$ in B_R, the functions u_k are locally uniformly Lipschitz and bounded and thus converge locally uniformly to some u_∞. The right-hand sides $\det D^2 u_k$ converge weakly to $\det D^2 u_\infty$ (see [Gutiérrez 2001]), so

$$\det D^2 u_\infty < \Lambda < \infty$$

in all of $\mathbb{R}^2$.

Finally, let

$$u(x_1, x_2) = u_\infty((|x_1| - 1)_+, x_2)$$

be the function obtained by translating u_∞ to the right and reflecting over the x_2-axis.

It is clear that u is even in x_1 and x_2, and is a one-dimensional function $f(x_2)$ in the strip $\{|x_1| < 1\}$. It is easy to show that f' is the standard Cantor function (appropriately rescaled), so f'' has a nontrivial Cantor part. Indeed, $\partial_2 u_k(0, \cdot)$ jumps by 2^{1-k} over each of 2^{k+1} intervals of length $3^{-(k+1)}$ centered at the endpoints of the sets removed in the construction of the Cantor set. By (4) we also have

$$u(\pm 2, 0) > u(0, 0) + \mu.$$

Since u is even over both axes we conclude that

$$\{u < u(0, 0) + \mu\} \subset [-2, 2] \times [-C, C].$$

By convexity, u has bounded sublevel sets, completing the proof. □

4. A propagation result

In $\mathbb{R}^2$, the second derivatives of a solution to (1) cannot concentrate on a single line segment, since Lipschitz singularities propagate. (Compare to the example above, where the second derivatives concentrate on a family of horizontal rays.) In this section we investigate more closely how solutions to (1) can behave near a single line segment in $\mathbb{R}^2$.

We first construct, for any $\epsilon > 0$, examples that grow from the origin like $|x_2|/|\log x_2|^{1+\epsilon}$, with $D^2 u$ not in $L \log^{1+\epsilon} L$. We then construct a family of barriers related to these examples in the case $\epsilon = 0$. Finally, we use these barriers to prove that singularities of the form $|x_2|/|\log x_2|$ propagate.

Examples that grow logarithmically slower than Lipschitz.

Proposition 4.1. *For any $\alpha > 0$ there exists a solution to* (1) *in two dimensions that vanishes at* 0 *and lies above $c|x_2|/|\log x_2|^{1+1/\alpha}$, and whose Hessian is not in $L \log^{1+1/\alpha} L$.*

Proof. Let $\Omega_1 = \{|x_2| < h(x_1)e^{-1/x_1^\alpha}\}$ for some positive even function h to be determined. (By x^γ we mean $|x|^\gamma$). In Ω_1, define

$$u_0(x_1, x_2) = x_1^{\alpha+1} e^{-1/x_1^\alpha} + x_1^{\alpha+1} e^{1/x_1^\alpha} x_2^2.$$

We would like to glue this to a function of x_2 on $\Omega_2 = \mathbb{R}^2 \setminus \Omega_1$, which imposes the condition $\partial_1 u_0 = 0$ on the boundary. Computing, we find that

$$h^2(t) = \frac{1+(\alpha+1)t^\alpha/\alpha}{1-(\alpha+1)t^\alpha/\alpha} = 1 + 2\frac{\alpha+1}{\alpha} t^\alpha + O(t^{2\alpha}).$$

In this way we ensure that u_0 glues in a C^1 manner across $\partial\Omega_1$ to some function $g(|x_2|)$ in Ω_2 defined by

$$g(h(t)e^{-1/t^\alpha}) = t^{\alpha+1}(1 + h^2(t))e^{-1/t^\alpha}.$$

The agreement of derivatives on $\partial\Omega_1$ gives

$$g'(h(t)e^{-1/t^\alpha}) = 2t^{\alpha+1}h(t),$$

which upon differentiation and using the formula for h gives

$$g''(h(t)e^{-1/t^\alpha}) = 2(1+1/\alpha+o(1))e^{1/t^\alpha}t^{2\alpha+1}.$$

For $|z|$ small it follows that

$$g''(z) \geq \frac{1}{|z|\,|\log z|^{2+1/\alpha}},$$

giving the nonintegrability claimed (after, say, replacing x_1 by $(|x_1|-1)_+$).

It remains to show that $\det D^2u_0$ is positive and bounded. One computes for

$$x_2^2 = s^2h(x_1)^2e^{-2/x_1^\alpha}, \quad s^2 < 1,$$

that

$$\det D^2u_0(x_1,x_2) = 2\alpha^2\big((1-s^2)+(\alpha+1)x_1^\alpha(1+s^2)/\alpha\big)+O(x_1^{2\alpha}),$$

completing the proof. □

Barriers. We now construct barriers that agree with $|x_2|/|\log x_2|$ except for in very thin cusps around the x_1-axis where the Monge–Ampère measure is as large as we like. Let

$$h_\alpha(t) = \begin{cases} 0, & t \leq 0, \\ \frac{1}{2}e^{-1/t^\alpha}, & t > 0, \end{cases}$$

where $\alpha > 0$ is large. Let $\Omega_{1,\alpha} = \{|x_2| < h_\alpha(x_1)\}$ be a thin cusp around the positive x_1-axis and let $\Omega_{2,\alpha}$ be its complement. Our barrier is

$$b_\alpha(x_1,x_2) = \begin{cases} x_1^\alpha e^{-1/x_1^\alpha} + x_1^\alpha e^{1/x_1^\alpha}x_2^2 & \text{in } \Omega_{1,\alpha}, \\ \frac{5}{2}|x_2|/|\log 2x_2| & \text{in } \Omega_{2,\alpha}. \end{cases}$$

Note that b_α is convex and bounded by 1 on $\Omega_{2,\alpha}\cap\{|x_2| < \frac{1}{4}\}$, and b_α is continuous across $\partial\Omega_{1,\alpha}$. Furthermore, on $\partial\Omega_{1,\alpha}$ one computes (from inside $\Omega_{1,\alpha}$) that

$$\partial_1 b_\alpha(x_1,x_2) = \alpha e^{-1/x_1^\alpha}\big(\tfrac{3}{4}x_1^{-1} + \tfrac{5}{4}x_1^{\alpha-1}\big) \geq 0,$$

so the derivatives have positive jumps across $\partial\Omega_{1,\alpha}$.

Set $x_2^2e^{2/x_1^\alpha} = a$. One computes in $\Omega_{1,\alpha}$ (where $a \leq \frac{1}{4}$) that

$$\begin{aligned} \det D^2b_\alpha &= 2\alpha^2x_1^{-2}\left((1-a) + \frac{\alpha-1+a(3\alpha+1)}{\alpha}x_1^\alpha + \frac{\alpha-1-a(\alpha+1)}{\alpha}x_1^{2\alpha}\right) \\ &\geq \tfrac{3}{2}\alpha^2x_1^{-2}. \end{aligned}$$

Finally, let $\Omega := \big(-\infty, \frac{1}{2}\big] \times \big[-\frac{1}{4}, \frac{1}{4}\big]$. We conclude that b_α are convex in Ω, with

$$\det D^2b_\alpha \geq 6\alpha^2 \quad \text{in } \Omega_{1,\alpha}\cap\Omega,$$

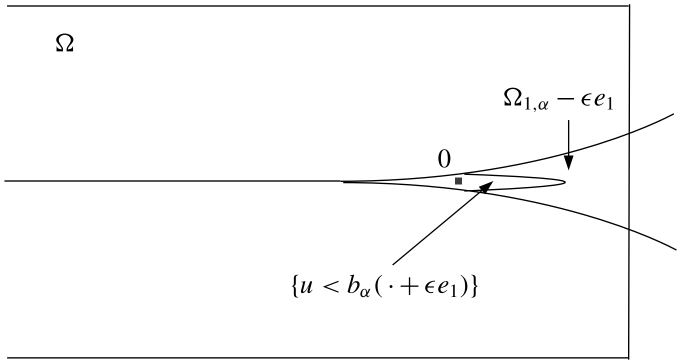

Figure 4. If $u > b_\alpha$ on the right edge of $\overline{\Omega_{1,\alpha}} \cap \Omega$, then we get a contradiction by sliding b_α to the left.

and furthermore

$$b_\alpha < \tfrac{5}{4} \cdot 2^{-\alpha} e^{-2^\alpha} \quad \text{for } \Omega_{1,\alpha} \cap \Omega.$$

Propagation. We prove Theorem 1.4 by sliding the barriers b_α from the right.

Proof of Theorem 1.4. By rescaling and multiplying by a constant, we may assume that

$$u \geq \tfrac{5}{2}|x_2|/|\log 2x_2| \quad \text{in } \left\{|x_2| < \tfrac{1}{4}\right\} \cap B_1,$$

with $u(0) = 0$ and $\det D^2 u < \Lambda$ for some large Λ. Choose α so large that $\alpha^2 > \Lambda$. Slide the barriers $b_\alpha(\cdot - te_1)$ from the right. Since $u \geq b_\alpha(\cdot - te_1)$ on $\partial(\Omega_{1,\alpha} + te_1) \cap \Omega$ for all $|t|$ small, it follows from the maximum principle that

$$u\left(\tfrac{1}{2}, x_2\right) \leq b_\alpha\left(\tfrac{1}{2}, x_2\right)$$

for some $\left(\tfrac{1}{2}, x_2\right) \in \overline{\Omega_{1,\alpha}} \cap \Omega$. (Indeed, if not, we can take $t = -\epsilon$ small and obtain

$$\{u < b_\alpha(\cdot + \epsilon e_1)\} \subset (\Omega_{1,\alpha} - \epsilon e_1) \cap \Omega,$$

which contradicts the Alexandrov maximum principle; see Figure 4). Taking $\alpha \to \infty$, we conclude that $u(e_1/2) = 0$.

By convexity, near each point on the x_1-axis where u is zero, there is a singularity of the same type as near the origin. We can apply the above argument at all such points to complete the proof. □

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References

[Alexandrov 1942] A. Alexandroff, "Smoothness of the convex surface of bounded Gaussian curvature", *C. R.* (*Doklady*) *Acad. Sci. URSS* (*N.S.*) **36** (1942), 195–199. MR 0007626 Zbl 0061.37605

[Ambrosio et al. 2012] L. Ambrosio, M. Colombo, G. De Philippis, and A. Figalli, "Existence of Eulerian solutions to the semigeostrophic equations in physical space: the 2-dimensional periodic case", *Comm. Partial Differential Equations* **37**:12 (2012), 2209–2227. MR 3005541 Zbl 1258.35164

[Ambrosio et al. 2014] L. Ambrosio, M. Colombo, G. De Philippis, and A. Figalli, "A global existence result for the semigeostrophic equations in three dimensional convex domains", *Discrete Contin. Dyn. Syst.* **34**:4 (2014), 1251–1268. MR 3117839 Zbl 1287.35064

[Daskalopoulos and Savin 2009] P. Daskalopoulos and O. Savin, "On Monge–Ampère equations with homogeneous right-hand sides", *Comm. Pure Appl. Math.* **62**:5 (2009), 639–676. MR 2494810 Zbl 1171.35341

[De Philippis and Figalli 2013] G. De Philippis and A. Figalli, "$W^{2,1}$ regularity for solutions of the Monge–Ampère equation", *Invent. Math.* **192**:1 (2013), 55–69. MR 3032325 Zbl 1286.35107

[De Philippis and Figalli 2014] G. De Philippis and A. Figalli, "The Monge–Ampère equation and its link to optimal transportation", *Bull. Amer. Math. Soc.* (*N.S.*) **51**:4 (2014), 527–580. MR 3237759

[De Philippis et al. 2013] G. De Philippis, A. Figalli, and O. Savin, "A note on interior $W^{2,1+\varepsilon}$ estimates for the Monge–Ampère equation", *Math. Ann.* **357**:1 (2013), 11–22. MR 3084340 Zbl 1280.35153

[Figalli 2015] A. Figalli, "Global existence for the semigeostrophic equations via Sobolev estimates for Monge–Ampère", lecture notes from CIME Summer Course on *Partial differential equations and geometric measure theory* (Cetraro, 2014), 2015, Available at http://cvgmt.sns.it/paper/2665/.

[Figalli and Loeper 2009] A. Figalli and G. Loeper, "C^1 regularity of solutions of the Monge–Ampère equation for optimal transport in dimension two", *Calc. Var. Partial Differential Equations* **35**:4 (2009), 537–550. MR 2496656 Zbl 1170.35400

[Guan 1997] P. Guan, "Regularity of a class of quasilinear degenerate elliptic equations", *Adv. Math.* **132**:1 (1997), 24–45. MR 1488238 Zbl 0892.35036

[Gutiérrez 2001] C. E. Gutiérrez, *The Monge–Ampère equation*, Progress in Nonlinear Differential Equations and their Applications **44**, Birkhäuser, Boston, 2001. MR 1829162 Zbl 0989.35052

[Schmidt 2013] T. Schmidt, "$\mathrm{W}^{2,1+\varepsilon}$ estimates for the Monge–Ampère equation", *Adv. Math.* **240** (2013), 672–689. MR 3046322 Zbl 1290.35136

[Wang 1995] X. J. Wang, "Some counterexamples to the regularity of Monge–Ampère equations", *Proc. Amer. Math. Soc.* **123**:3 (1995), 841–845. MR 1223269 Zbl 0822.35054

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MEAN ERGODIC THEOREM FOR AMENABLE DISCRETE QUANTUM GROUPS AND A WIENER-TYPE THEOREM FOR COMPACT METRIZABLE GROUPS

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We prove a mean ergodic theorem for amenable discrete quantum groups. As an application, we prove a Wiener-type theorem for continuous measures on compact metrizable groups.

1. Introduction

A countable discrete group Γ is called *amenable* if there exists a sequence $\{F_n\}_{n=1}^{\infty}$ (called a right Følner sequence) consisting of finite subsets F_n of Γ such that

$$\lim_{n\to\infty} \frac{1}{|F_n|} |F_n s \Delta F_n| = 0$$

for every $s \in \Gamma$.

Let $(X, \mathscr{B}, \mu, \Gamma)$ be a dynamical system consisting of a countable discrete amenable group Γ with a measure-preserving action on a probability space $(X, \mathscr{B}, \mu)$.

Recall that von Neumann's mean ergodic theorem for amenable group actions on measure spaces says the following:

Theorem 1.1 (measure space version of von Neumann's mean ergodic theorem [Glasner 2003, Theorem 3.33]). *Let $\{F_n\}_{n=1}^{\infty}$ be a right Følner sequence of Γ. Then, for every $f \in L^2(X, \mu)$, the sequence $(1/|F_n|)\sum_{s\in F_n} s \cdot f$ converges to Pf with respect to the L^2 norm, where P is the orthogonal projection from $L^2(X, \mu)$ onto the space $\{g \in L^2(X, \mu) \mid s \cdot g = g$ for all $s \in \Gamma\}$.*

R. Duvenhage [2008, Theorem 3.1] proves a generalization of von Neumann's mean ergodic theorem for coactions of amenable quantum groups on von Neumann algebras (noncommutative measure spaces). Later, a more general version was proved by V. Runge and A. Viselter [2014, Theorem 2.2].

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There is also a version of von Neumann's mean ergodic theorem for amenable group actions on Hilbert spaces, which says the following:

Theorem 1.2 (Hilbert space version of von Neumann's mean ergodic theorem). *Let $\{F_n\}_{n=1}^{\infty}$ be a right Følner sequence of a countable discrete amenable group Γ and $\pi : \Gamma \to B(H)$ be a unitary representation of Γ on a Hilbert space H. Set $H_\Gamma = \{x \in H \mid \pi(s)x = x \text{ for all } s \in \Gamma\}$. Then*

$$\lim_{n\to\infty} \frac{1}{|F_n|} \sum_{s\in F_n} \pi(s) = P$$

under the strong operator topology on $B(H)$, where P is the orthogonal projection from H onto H_Γ.

The group C^*-algebra $C^*(\Gamma)$ equals $C(G)$ for a coamenable compact quantum group G with the dual group $\widehat{G} = \Gamma$. The counit ε of G is given by $\varepsilon(\delta_s) = 1$ for all $s \in \Gamma$. Hence,

$$H_\Gamma = \{x \in H \mid \pi(a)x = \varepsilon(a)x \ \text{ for all } \ a \in C^*(\Gamma)\}.$$

With these in mind, the Hilbert space version of von Neumann's mean ergodic theorem can be reformulated in the framework of compact quantum groups as follows.

Suppose G is a coamenable compact quantum group such that the dual $\widehat{G}$ is a countable discrete amenable group Γ. Let $\{F_n\}_{n=1}^{\infty}$ be a right Følner sequence of Γ and $\pi : C(G) = C^*(\Gamma) \to B(H)$ be a representation of $C^*(\Gamma)$ on a Hilbert space H. Then

$$\lim_{n\to\infty} \frac{1}{|F_n|} \sum_{s\in F_n} \pi(s) = P$$

under the strong operator topology on $B(H)$, where P is the orthogonal projection from H onto $H_\Gamma = \{x \in H \mid \pi(a)x = \varepsilon(a)x \text{ for all } a \in C^*(\Gamma)\}$.

D. Kyed proves that a compact quantum group G is coamenable if and only if there exists a right Følner sequence $\{F_n\}_{n=1}^{\infty}$ of finite subsets in its dual $\widehat{G}$, that is to say, G is a coamenable compact quantum group if and only if $\widehat{G}$ is an amenable discrete quantum group [2008, Definition 4.9.].[1] So it is natural to ask for a generalization of the Hilbert space version of von Neumann's mean ergodic theorem to all amenable discrete quantum groups. This is the main result of the paper.

Theorem 3.1 (mean ergodic theorem for amenable discrete quantum groups). *Let G be a coamenable compact quantum group with counit ε and let $\{F_n\}_{n=1}^{\infty}$ be a right Følner sequence of $\widehat{G}$. Set $H_{\text{inv}} = \{x \in H \mid \pi(a)x = \varepsilon(a)x \text{ for all } a \in A\}$. For a representation $\pi : A = C(G) \to B(H)$, we have*

$$\lim_{n\to\infty} \frac{1}{|F_n|_w} \sum_{\alpha\in F_n} d_\alpha \pi(\chi(\alpha)) = P \tag{1-1}$$

under the strong operator topology, where P is the orthogonal projection from H onto H_{inv}.

[1] The existence of a Følner sequence for Kac-type compact quantum groups is shown by Z. Ruan [1996]. Also see [Tomatsu 2006].

Here $|F_n|_w$ stands for the weighted cardinality of F_n. Definitions of $|F_n|_w$, d_α and $\chi(\alpha)$ are in Section 2.

The left-hand side of (1-1) involves both a representation of a coamenable compact quantum group G and that of its discrete quantum group dual $\widehat{G}$, so it illustrates some interactions between them.

The rest of the paper aims at an application of Theorem 3.1. Namely, we prove a Wiener-type theorem for finite Borel measures on compact metrizable groups.

A finite Borel measure μ on a compact metrizable space X is called *continuous* or *nonatomic* if $\mu\{x\} = 0$ for every $x \in X$.

The following theorem of N. Wiener [1933] expresses finite Borel measures on the unit circle via their Fourier coefficients.

Theorem 1.3 (Wiener's theorem [Katznelson 2004, Chapter 1, Theorem 7.13]). *For a finite Borel measure μ on the unit circle $\mathbb{T}$ and every $z \in \mathbb{T}$, one has*

$$\lim_{N\to\infty} \frac{1}{2N+1} \sum_{n=-N}^{N} \hat{\mu}(n) z^{-n} = \mu\{z\} \quad \textit{and} \quad \lim_{N\to\infty} \frac{1}{2N+1} \sum_{n=-N}^{N} |\hat{\mu}(n)|^2 = \sum_{x\in\mathbb{T}} \mu\{x\}^2.$$

Hence, μ is continuous if and only if

$$\lim_{N\to\infty} \frac{1}{2N+1} \sum_{n=-N}^{N} |\hat{\mu}(n)|^2 = 0,$$

where $\hat{\mu}(n) := \int_{\mathbb{T}} z^n \, d\mu(z)$ for $n \in \mathbb{Z}$ are the Fourier coefficients of μ.

There are various generalized Wiener's theorems (we call such generalizations Wiener-type theorems), including a version for compact manifolds [Taylor 1981, Chapter XII, Theorem 5.1], a version for compact Lie groups by M. Anoussis and A. Bisbas [2000, Theorem 7], and a version for compact homogeneous manifolds by M. Björklund and A. Fish [2009, Lemma 2.1].

We apply the above mean ergodic theorem (Theorem 3.1) to get a Wiener-type theorem on compact metrizable groups. This version differs from previous ones mainly in two aspects: firstly we don't require smoothness on spaces; secondly we use a different Følner condition.

Theorem 4.1 (Wiener-type theorem for compact metrizable groups). *Let G be a compact metrizable group. Given y in G and a right Følner sequence $\{F_n\}_{n=1}^{\infty}$ of $\widehat{G}$, for a finite Borel measure μ on G one has*

$$\lim_{n\to\infty} \frac{1}{|F_n|_w} \sum_{\alpha\in F_n} d_\alpha \sum_{1\le i,j\le d_\alpha} \mu(u_{ij}^{\alpha}) \overline{u_{ij}^{\alpha}(y)} = \mu\{y\} \quad \textit{and} \quad \lim_{n\to\infty} \frac{1}{|F_n|_w} \sum_{\alpha\in F_n} d_\alpha \sum_{1\le i,j\le d_\alpha} |\mu(u_{ij}^{\alpha})|^2 = \sum_{x\in G} \mu\{x\}^2.$$

Hence, μ is continuous if and only if

$$\lim_{n\to\infty} \frac{1}{|F_n|_w} \sum_{\alpha\in F_n} d_\alpha \sum_{1\le i,j\le d_\alpha} |\mu(u_{ij}^{\alpha})|^2 = 0.$$

Here the u_{ij}^{α} are the matrix coefficients of the irreducible unitary representation α of G; see Section 2 for the precise definition.

The paper is organized as follows.

In Section 2, we collect some basic facts in compact quantum group theory. In Section 3, we prove the mean ergodic theorem, i.e., Theorem 3.1. As a consequence, we obtain Corollary 3.7, which is used in Section 4 to prove Theorem 4.1.

2. Preliminaries

Conventions. Within this paper, we use $B(H, K)$ to denote the space of bounded linear operators from a Hilbert space H to another Hilbert space K, and $B(H)$ stands for $B(H, H)$.

A net $\{T_\lambda\} \subset B(H)$ converges to $T \in B(H)$ under the strong operator topology (SOT) if $T_\lambda x \to Tx$ for every $x \in H$, and $\{T_\lambda\}$ converges to $T \in B(H)$ under the weak operator topology (WOT) if $\langle T_\lambda x, y\rangle \to \langle Tx, y\rangle$ for all $x, y \in H$.

The notation $A \otimes B$ always means the minimal tensor product of two C^*-algebras A and B.

For a state φ on a unital C^*-algebra A, we use $L^2(A, \varphi)$ to denote the Hilbert space of Gelfand–Neimark–Segal (GNS) representations of A with respect to φ. The image of $a \in A$ in $L^2(A, \varphi)$ is denoted by $\hat{a}$.

In this paper all C^*-algebras are assumed to be unital and separable.

Some facts about compact quantum groups. Compact quantum groups are noncommutative analogues of compact groups. They were introduced by S. L. Woronowicz [1987; 1998].

Definition 2.1. A *compact quantum group* is a pair (A, Δ) consisting of a unital C^*-algebra A and a unital $*$-homomorphism

$$\Delta : A \to A \otimes A$$

such that

(1) $(\mathrm{id} \otimes \Delta)\Delta = (\Delta \otimes \mathrm{id})\Delta$;

(2) $\Delta(A)(1 \otimes A)$ and $\Delta(A)(A \otimes 1)$ are dense in $A \otimes A$.

One may think of A as $C(G)$, the C^*-algebra of continuous functions on a compact quantum space G with a quantum group structure. In the rest of the paper we write a compact quantum group (A, Δ) as G. The $*$-homomorphism Δ is called the *coproduct* of G.

There exists a unique state h on A such that

$$(h \otimes \mathrm{id})\Delta(a) = (\mathrm{id} \otimes h)\Delta(a) = h(a)1_A$$

for all a in A. The state h is called the *Haar measure* of G. Throughout this paper, we use h to denote it.

For a compact quantum group G, there is a unique dense unital $*$-subalgebra $\mathscr{A}$ of A such that:

(1) Δ maps from $\mathscr{A}$ to $\mathscr{A} \odot \mathscr{A}$ (the algebraic tensor product).

(2) There exists a unique multiplicative linear functional $\varepsilon : \mathscr{A} \to \mathbb{C}$ and a linear map $\kappa : \mathscr{A} \to \mathscr{A}$ such that $(\varepsilon \otimes \mathrm{id})\Delta(a) = (\mathrm{id} \otimes \varepsilon)\Delta(a) = a$ and $m(\kappa \otimes \mathrm{id})\Delta(a) = m(\mathrm{id} \otimes \kappa)\Delta(a) = \varepsilon(a)1$ for all $a \in \mathscr{A}$, where $m : \mathscr{A} \odot \mathscr{A} \to \mathscr{A}$ is the multiplication map. The functional ε is called the *counit* and κ the *coinverse* of $C(G)$.

Note that ε is only densely defined and not necessarily bounded. If ε is bounded and h is faithful ($h(a^*a) = 0$ implies $a = 0$), then G is called *coamenable* [Bédos et al. 2001]. Examples of coamenable compact quantum groups include $C(G)$ for a compact group G and $C^*(\Gamma)$ for a discrete amenable group Γ.

A nondegenerate (unitary) *representation* U of a compact quantum group G is an invertible (unitary) element in $M(K(H) \otimes A)$ for some Hilbert space H satisfying that $U_{12}U_{13} = (\mathrm{id} \otimes \Delta)U$. Here $K(H)$ is the C^*-algebra of compact operators on H and $M(K(H) \otimes A)$ is the multiplier C^*-algebra of $K(H) \otimes A$.

We write U_{12} and U_{13}, respectively, for the images of U by two maps from $M(K(H) \otimes A)$ to $M(K(H) \otimes A \otimes A)$, where the first one is obtained by extending the map $x \mapsto x \otimes 1$ from $K(H) \otimes A$ to $K(H) \otimes A \otimes A$, and the second one is obtained by composing this map with the flip on the last two factors. The Hilbert space H is called the *carrier Hilbert space* of U. From now on, we always assume representations are nondegenerate. If the carrier Hilbert space H is of finite dimension, then U is called a finite-dimensional representation of G.

For two representations U_1 and U_2 with the carrier Hilbert spaces H_1 and H_2, respectively, the set of *intertwiners* between U_1 and U_2, $\mathrm{Mor}(U_1, U_2)$, is defined by

$$\mathrm{Mor}(U_1, U_2) = \{T \in B(H_1, H_2) \mid (T \otimes 1)U_1 = U_2(T \otimes 1)\}.$$

Two representations U_1 and U_2 are equivalent if there exists a bijection T in $\mathrm{Mor}(U_1, U_2)$. A representation U is called *irreducible* if $\mathrm{Mor}(U, U) \cong \mathbb{C}$.

Moreover, we have the following well-established facts about representations of compact quantum groups:

(1) Every finite-dimensional representation is equivalent to a unitary representation.

(2) Every irreducible representation is finite-dimensional.

Let $\widehat{G}$ be the set of equivalence classes of irreducible unitary representations of G. For every $\gamma \in \widehat{G}$, let $U^\gamma \in \gamma$ be unitary and H_γ be its carrier Hilbert space with dimension d_γ. After fixing an orthonormal basis of H_γ, we can write U^γ as $(u^\gamma_{ij})_{1 \le i, j \le d_\gamma}$ with $u^\gamma_{ij} \in A$, and

$$\Delta(u^\gamma_{ij}) = \sum_{k=1}^{d_\gamma} u^\gamma_{ik} \otimes u^\gamma_{kj}$$

for all $1 \le i,\, j \le d_\gamma$.

The matrix $\overline{U^\gamma}$ is still an irreducible representation (not necessarily unitary) with the carrier Hilbert space $\overline{H}_\gamma$. It is called the *conjugate* representation of U^γ and the equivalence class of $\overline{U^\gamma}$ is denoted by $\overline{\gamma}$.

Given two finite-dimensional representations α and β of G, fix orthonormal bases for α and β and write α and β as U^α and U^β in matrix forms, respectively. Define the *direct sum*, denoted by $\alpha + \beta$, as the equivalence class of unitary representations of dimension $d_\alpha + d_\beta$ given by

$$\begin{pmatrix} U^\alpha & 0 \\ 0 & U^\beta \end{pmatrix},$$

and the *tensor product*, denoted by $\alpha\beta$, is the equivalence class of unitary representations of dimension $d_\alpha d_\beta$ whose matrix form is given by $U^{\alpha\beta} = U^\alpha_{13} U^\beta_{23}$.

The *character* $\chi(\alpha)$ of a finite-dimensional representation α is given by

$$\chi(\alpha) = \sum_{i=1}^{d_\alpha} u^\alpha_{ii}.$$

Note that $\chi(\alpha)$ is independent of the choice of representatives of α. Also we have $\|\chi(\alpha)\| \le d_\alpha$, since $\sum_{k=1}^{d_\alpha} u^\alpha_{ik}(u^\alpha_{ik})^* = 1$ for every $1 \le i \le d_\alpha$. Moreover,

$$\chi(\alpha+\beta) = \chi(\alpha) + \chi(\beta), \quad \chi(\alpha\beta) = \chi(\alpha)\chi(\beta) \quad \text{and} \quad \chi(\alpha)^* = \chi(\bar{\alpha})$$

for finite-dimensional representations α and β.

Every representation of a compact quantum group is a direct sum of irreducible representations. For two finite-dimensional representations α and β, denote by $N^\gamma_{\alpha,\beta}$ the number of copies of $\gamma \in \widehat{G}$ in the decomposition of $\alpha\beta$ into a sum of irreducible representations. Hence,

$$\alpha\beta = \sum_{\gamma \in \widehat{G}} N^\gamma_{\alpha,\beta}\gamma.$$

We have the Frobenius reciprocity law [Woronowicz 1987, Proposition 3.4; Kyed 2008, Example 2.3]

$$N^\gamma_{\alpha,\beta} = N^\alpha_{\gamma,\bar{\beta}} = N^\beta_{\bar{\alpha},\gamma}$$

for all $\alpha, \beta, \gamma \in \widehat{G}$.

Throughout, we assume that $A = C(G)$ is a separable C^*-algebra, which amounts to saying $\widehat{G}$ is countable.

Definition 2.2 [Kyed 2008, Definition 3.2]. Given two finite subsets S and F of $\widehat{G}$, the *boundary* of F relative to S, denoted by $\partial_S(F)$, is defined by

$$\partial_S(F) = \{\alpha \in F \mid N^\beta_{\alpha,\gamma} > 0 \text{ for some } \gamma \in S,\ \beta \notin F\} \cup \{\alpha \notin F \mid N^\beta_{\alpha,\gamma} > 0 \text{ for some } \gamma \in S,\ \beta \in F\}.$$

The *weighted cardinality* $|F|_w$ of a finite subset F of $\widehat{G}$ is given by

$$|F|_w = \sum_{\alpha \in F} d^2_\alpha.$$

D. Kyed proves a compact quantum group G is coamenable if and only if there exists a Følner sequence in $\widehat{G}$.

Theorem 2.3 (Følner condition for amenable discrete quantum groups [Kyed 2008, Corollary 4.10]). *A compact quantum group G is coamenable if and only if there exists a sequence $\{F_n\}_{n=1}^\infty$ (a right Følner sequence) of finite subsets of $\widehat{G}$ such that*

$$\lim_{n\to\infty} \frac{|\partial_S(F_n)|_w}{|F_n|_w} = 0$$

for every finite nonempty subset S of $\widehat{G}$.

3. Mean ergodic theorem for amenable discrete quantum groups

In this section we prove the generalized mean ergodic theorem.

Theorem 3.1. *Let G be a coamenable compact quantum group with counit ε and $\{F_n\}_{n=1}^{\infty}$ be a right Følner sequence of $\widehat{G}$. For a representation $\pi : A = C(G) \to B(H)$, we have*

$$\lim_{n\to\infty} \frac{1}{|F_n|_w} \sum_{\alpha\in F_n} d_\alpha \pi(\chi(\alpha)) = P \tag{3-1}$$

under the strong operator topology, where P is the orthogonal projection from H onto

$$H_{\text{inv}} = \{x \in H \mid \pi(a)x = \varepsilon(a)x \text{ for all } a \in A\}.$$

We divide the proof into two major steps:

Step 1. *We show that $H_{\text{inv}} = K$ for $K = \{x \in H \mid \pi(\chi(\alpha))x = d_\alpha x$ for all $\alpha \in \widehat{G}\}$.*

Step 2. *The sequence $\bigl\{(1/|F_n|_w)\sum_{\alpha\in F_n} d_\alpha\pi(\chi(\alpha))\bigr\}_{n=1}^{\infty}$ converges to the projection from H onto K.*

Proof of Step 1 for Theorem 3.1. We proceed via two lemmas:

Lemma 3.2. *If a state φ on $A = C(G)$ for a compact quantum group G satisfies that $\varphi(\chi(\alpha)) = d_\alpha$ for all $\alpha \in \widehat{G}$, then $\varphi = \varepsilon$.*

Proof. It suffices to show that $\varphi(u_{ij}^{\alpha}) = \delta_{ij}$ for every $\alpha \in \widehat{G}$ and an arbitrary unitary $U = (u_{ij}^{\alpha})_{1\le i,j\le d_\alpha} \in \alpha$.

Let $\varphi(U)$ be the matrix $(\varphi(u_{ij}^{\alpha}))$ in $M_{d_\alpha}(\mathbb{C})$. Note that φ is a state, hence completely positive. By a generalized Schwarz inequality of M. Choi [1974, Corollary 2.8], we have

$$\varphi(U)\varphi(U^*) \le \varphi(UU^*) = 1.$$

Let Tr be the normalized trace of $M_{d_\alpha}(\mathbb{C})$. Since $\varphi(\chi(\alpha)) = d_\alpha$, we get $\mathrm{Tr}(\varphi(U)) = 1$. It follows that

$$\begin{aligned}
0 &\le \mathrm{Tr}\bigl((\varphi(U)-1)(\varphi(U)-1)^*\bigr)\\
&= \mathrm{Tr}(\varphi(U)\varphi(U)^* - \varphi(U)^* - \varphi(U) + 1)\\
&= \mathrm{Tr}(\varphi(U)\varphi(U)^*) - 1\\
&= \mathrm{Tr}(\varphi(U)\varphi(U^*)) - 1\\
&\le \mathrm{Tr}(\varphi(UU^*)) - 1 = 0.
\end{aligned}$$

Hence, $\mathrm{Tr}\bigl((\varphi(U)-1)(\varphi(U)-1)^*\bigr) = 0$, which implies that $\varphi(U) = 1$. This ends the proof. □

Lemma 3.3. *Let $\pi : A = C(G) \to B(H)$ be a representation. Then*

$$H_{\text{inv}} = K = \{x \in H \mid \pi(\chi(\alpha))x = d_\alpha x \text{ for all } \alpha \in \widehat{G}\}.$$

Proof. Note that $\varepsilon(\chi(\alpha)) = d_\alpha$ for all $\alpha \in \widehat{G}$ [Woronowicz 1998, Formula (5.11)]. Hence $H_{\text{inv}} \subseteq K$.

To show $K \subseteq H_{\text{inv}}$, we can assume $K \ne 0$ without loss of generality.

Let $x \in K$ be an arbitrarily chosen unit vector. By Lemma 3.2, the state φ_x defined by $\varphi_x(a) = \langle \pi(a)x, x\rangle$ for all $a \in A$ is ε, since $\varphi_x(\chi(\alpha)) = d_\alpha$ for all $\alpha \in \widehat{G}$.

For every $a \in A$, we have

$$\begin{aligned}\|\pi(a)x - \varepsilon(a)x\|^2 &= \langle \pi(a)x - \varepsilon(a)x, \pi(a)x - \varepsilon(a)x\rangle \\ &= \langle \pi(a)x, \pi(a)x\rangle - \langle \varepsilon(a)x, \pi(a)x\rangle - \langle \pi(a)x, \varepsilon(a)x\rangle + \langle \varepsilon(a)x, \varepsilon(a)x\rangle \\ &= \langle \pi(a^*a)x, x\rangle - \langle \varepsilon(a)\pi(a^*)x, x\rangle - \overline{\varepsilon(a)}\langle \pi(a)x, x\rangle + |\varepsilon(a)|^2 \\ &= \varepsilon(a^*a) - \varepsilon(a)\varepsilon(a^*) - |\varepsilon(a)|^2 + |\varepsilon(a)|^2 \\ &= 0.\end{aligned}$$

This proves that $K \subseteq H_{\text{inv}}$, and so concludes the proof of Step 1. □

Proof of Step 2 for Theorem 3.1. We start with a lemma:

Lemma 3.4. *The orthogonal complement $H_{\text{inv}}^{\perp}$ of H_{inv} is*

$$V := \overline{\operatorname{Span}\big\{\pi(\chi(\alpha))x - d_\alpha x \mid \alpha \in \widehat{G},\ x \in H\big\}}.$$

We need the following well-known fact in functional analysis:

Proposition 3.5. *Suppose $\{T_j\}_{j\in J}$ is a family of bounded operators on a Hilbert space H. Then the orthogonal complement of $\bigcap_{j\in J} \ker T_j$ is*

$$\overline{\operatorname{ran}\{T_j^* \mid j \in J\}},$$

the closed linear span of the ranges $\operatorname{ran} T_j^*$ *of T_j^* for all j in J.*

Proof of Lemma 3.4. Consider the family of operators $\{\pi(\chi(\alpha)) - d_\alpha\}_{\alpha\in\widehat{G}}$ in $B(H)$. These are self-adjoint operators, since

$$(\pi(\chi(\alpha)) - d_\alpha)^* = \pi(\chi(\overline{\alpha})) - d_{\overline{\alpha}},$$

Applying Proposition 3.5 to $\{\pi(\chi(\alpha)) - d_\alpha\}_{\alpha\in\widehat{G}}$ gives the proof. □

Now we are ready to finish the proof of Theorem 3.1.

For every $x \in H_{\text{inv}}$ and all n, we have

$$\frac{1}{|F_n|_w}\sum_{\alpha\in F_n} d_\alpha \pi(\chi(\alpha))x = \frac{1}{|F_n|_w}\sum_{\alpha\in F_n} d_\alpha^2 x = x.$$

Next we show that

$$\frac{1}{|F_n|_w}\sum_{\alpha\in F_n} d_\alpha \pi(\chi(\alpha))z \to 0$$

for all $z \in V$ as $n \to \infty$. By Lemma 3.4, we only need to prove it for z of the form $\pi(\chi(\gamma))y - d_\gamma y$ for every $y \in H$ and $\gamma \in \widehat{G}$.

For every $y \in H$ and $\gamma \in \widehat{G}$, we have

$$
\begin{aligned}
&\lim_{n\to\infty} \frac{1}{|F_n|_w} \sum_{\alpha\in F_n} d_\alpha \pi(\chi(\alpha))(\pi(\chi(\gamma))y - d_\gamma y) \\
&= \lim_{n\to\infty} \frac{1}{|F_n|_w}\Big(\sum_{\alpha\in F_n\setminus\partial_\gamma F_n} + \sum_{\alpha\in F_n\cap\partial_\gamma F_n}\Big) d_\alpha \pi(\chi(\alpha)\chi(\gamma))y - d_\alpha d_\gamma \pi(\chi(\alpha))y \\
&\hspace{18em}\text{(by Theorem 2.3 and since } \chi(\alpha)\chi(\gamma)=\chi(\alpha\gamma)) \\
&= \lim_{n\to\infty} \frac{1}{|F_n|_w} \sum_{\alpha\in F_n\setminus\partial_\gamma F_n} d_\alpha \pi(\chi(\alpha\gamma))y - d_\alpha d_\gamma \pi(\chi(\alpha))y \qquad \Big(\alpha\gamma = \sum_{\beta\in F_n} N^\beta_{\alpha,\gamma}\beta \text{ when } \alpha\in F_n\setminus\partial_\gamma F_n\Big) \\
&= \lim_{n\to\infty} \frac{1}{|F_n|_w}\Big(\sum_{\alpha\in F_n\setminus\partial_\gamma F_n}\sum_{\beta\in F_n} d_\alpha N^\beta_{\alpha,\gamma}\pi(\chi(\beta))y - \sum_{\alpha\in F_n\setminus\partial_\gamma F_n} d_\alpha d_\gamma \pi(\chi(\alpha))y\Big) \\
&\hspace{22em}(N^\beta_{\alpha,\gamma} = N^\alpha_{\beta,\overline{\gamma}} \text{ and } d_\gamma = d_{\overline{\gamma}}) \\
&= \lim_{n\to\infty} \frac{1}{|F_n|_w}\Big(\sum_{\alpha\in F_n\setminus\partial_\gamma F_n}\sum_{\beta\in F_n} d_\alpha N^\alpha_{\beta,\overline{\gamma}}\pi(\chi(\beta))y - \sum_{\alpha\in F_n\setminus\partial_\gamma F_n} d_\alpha d_{\overline{\gamma}} \pi(\chi(\alpha))y\Big) \\
&= \lim_{n\to\infty} \frac{1}{|F_n|_w}\Big(\sum_{\alpha\in F_n\setminus\partial_\gamma F_n}\sum_{\beta\in F_n} d_\alpha N^\alpha_{\beta,\overline{\gamma}}\pi(\chi(\beta))y - \sum_{\alpha\in F_n\setminus\partial_\gamma F_n}\Big[\sum_{\beta\in F_n} + \sum_{\beta\notin F_n}\Big] N^\beta_{\alpha,\overline{\gamma}} d_\beta \pi(\chi(\alpha))y\Big) \\
&\hspace{20em}\text{(exchange } \alpha \text{ and } \beta \text{ in the second term)} \\
&= \lim_{n\to\infty} \frac{1}{|F_n|_w}\Big(\sum_{\alpha\in F_n\setminus\partial_\gamma F_n}\sum_{\beta\in F_n} d_\alpha N^\alpha_{\beta,\overline{\gamma}}\pi(\chi(\beta))y - \sum_{\beta\in F_n\setminus\partial_\gamma F_n}\Big[\sum_{\alpha\in F_n} + \sum_{\alpha\notin F_n}\Big] N^\alpha_{\beta,\overline{\gamma}} d_\alpha \pi(\chi(\beta))y\Big) \\
&\hspace{22em}\text{(common terms are canceled)} \\
&= \lim_{n\to\infty} \frac{1}{|F_n|_w}\Big(\sum_{\alpha\in F_n\setminus\partial_\gamma F_n}\sum_{\beta\in F_n\cap\partial_\gamma F_n} d_\alpha N^\alpha_{\beta,\overline{\gamma}}\pi(\chi(\beta))y \\
&\qquad - \sum_{\beta\in F_n\setminus\partial_\gamma F_n}\sum_{\alpha\in F_n\cap\partial_\gamma F_n} N^\alpha_{\beta,\overline{\gamma}} d_\beta \pi(\chi(\beta))y - \sum_{\beta\in F_n\setminus\partial_\gamma F_n}\sum_{\alpha\notin F_n} N^\alpha_{\beta,\overline{\gamma}} d_\alpha \pi(\chi(\beta))y\Big) \\
&= 0.
\end{aligned}
$$

Note that the last equality above holds since, by Theorem 2.3, we have the following:

$$
\begin{aligned}
(1)\quad \frac{1}{|F_n|_w}\Big\|\sum_{\alpha\in F_n\setminus\partial_\gamma F_n}\sum_{\beta\in F_n\cap\partial_\gamma F_n} d_\alpha N^\alpha_{\beta,\overline{\gamma}}\pi(\chi(\beta))y\Big\| &\le \frac{1}{|F_n|_w}\sum_{\beta\in F_n\cap\partial_\gamma F_n}\sum_{\alpha\in F_n} d_\alpha N^\alpha_{\beta,\overline{\gamma}} d_\beta \|y\| \\
&\le \frac{1}{|F_n|_w}\sum_{\beta\in F_n\cap\partial_\gamma F_n} d_\beta^2 d_{\overline{\gamma}}\|y\| \to 0;
\end{aligned}
$$

$$
\begin{aligned}
(2)\quad \frac{1}{|F_n|_w}\Big\|\sum_{\beta\in F_n\setminus\partial_\gamma F_n}\sum_{\alpha\in F_n\cap\partial_\gamma F_n} N^\alpha_{\beta,\overline{\gamma}} d_\alpha\pi(\chi(\beta))y\Big\| &\le \frac{1}{|F_n|_w}\sum_{\beta\in F_n\setminus\partial_\gamma F_n}\sum_{\alpha\in F_n\cap\partial_\gamma F_n} N^\alpha_{\beta,\overline{\gamma}} d_\alpha d_\beta \|y\| \\
&= \frac{1}{|F_n|_w}\sum_{\beta\in F_n\setminus\partial_\gamma F_n}\sum_{\alpha\in F_n\cap\partial_\gamma F_n} N^\beta_{\alpha,\gamma} d_\alpha d_\beta \|y\| \\
&\le \frac{1}{|F_n|_w}\sum_{\alpha\in F_n\cap\partial_\gamma F_n} d_\alpha^2 d_\gamma \|y\| \to 0;
\end{aligned}
$$

$$(3)\quad \frac{1}{|F_n|_w}\Big\|\sum_{\beta\in F_n\setminus\partial_\gamma F_n}\sum_{\alpha\notin F_n}N^{\alpha}_{\beta,\bar{\gamma}}d_\alpha\pi(\chi(\beta))y\Big\| \le \frac{1}{|F_n|_w}\sum_{\beta\in F_n\setminus\partial_\gamma F_n}\sum_{\alpha\notin F_n}N^{\alpha}_{\beta,\bar{\gamma}}d_\alpha d_\beta\|y\|$$
$$= \frac{1}{|F_n|_w}\sum_{\beta\in F_n\setminus\partial_\gamma F_n}\sum_{\alpha\notin F_n,\, N^{\alpha}_{\beta,\bar{\gamma}}>0}N^{\alpha}_{\beta,\bar{\gamma}}d_\alpha d_\beta\|y\|$$
$$\le \frac{1}{|F_n|_w}\sum_{\beta\in\partial_{\bar{\gamma}} F_n}\sum_{\alpha\in\widehat{G}}N^{\alpha}_{\beta,\bar{\gamma}}d_\alpha d_\beta\|y\|$$
$$= \frac{1}{|F_n|_w}\sum_{\beta\in\partial_{\bar{\gamma}} F_n}d_\beta^2 d_{\bar{\gamma}}\|y\| \to 0 \quad \text{as } n\to\infty.$$

This completes proof of Step 2 and therefore of Theorem 3.1. □

For a representation $\pi : B \to B(H)$ of a unital C^*-algebra B, define the *commutant* $\pi(B)'$ of $\pi(B)$ by

$$\pi(B)' = \{T \in B(H) \mid T\pi(b) = \pi(b)T \ \text{ for all } \ b \in B\}.$$

Corollary 3.6. *In the setting of Theorem 3.1, the projection P is in $\pi(A)' \cap \overline{\pi(A)}^{\mathrm{SOT}}$.*

Proof. The left-hand side of (3-1) is in $\overline{\pi(A)}^{\mathrm{SOT}}$; hence, so is P. Moreover, for all $x, y \in H$ and $a \in A$, we have

$$\langle \pi(a)Px, y\rangle = \varepsilon(a)\langle Px, y\rangle$$

and

$$\langle P\pi(a)x, y\rangle = \langle \pi(a)x, Py\rangle = \langle x, \pi(a^*)Py\rangle = \langle x, \varepsilon(a^*)Py\rangle = \varepsilon(a)\langle Px, y\rangle.$$

This proves $P \in \pi(A)'$. □

As a consequence, we have the following:

Corollary 3.7. *Assume that φ is a pure state on $A = C(G)$ for a coamenable compact quantum group G and $\{F_n\}_{n=1}^{\infty}$ is a right Følner sequence of $\widehat{G}$. Then*

$$\lim_{n\to\infty}\frac{1}{|F_n|_w}\sum_{\alpha\in F_n}d_\alpha\varphi(\chi(\alpha)) = \begin{cases}1 & \text{if } \varphi = \varepsilon,\\ 0 & \text{if } \varphi \neq \varepsilon.\end{cases}$$

Proof. When $\varphi = \varepsilon$, we have $\varepsilon(\chi(\alpha)) = d_\alpha$ for all $\alpha \in \widehat{G}$ [Woronowicz 1998, Formula (5.11)]. Hence,

$$\lim_{n\to\infty}\frac{1}{|F_n|_w}\sum_{\alpha\in F_n}d_\alpha\varepsilon(\chi(\alpha)) = 1.$$

Suppose $\varphi \neq \varepsilon$.

Consider the GNS representation $\pi_\varphi : A \to B(L^2(A, \varphi))$. We have

$$\lim_{n\to\infty}\frac{1}{|F_n|_w}\sum_{\alpha\in F_n}d_\alpha\varphi(\chi(\alpha)) = \lim_{n\to\infty}\frac{1}{|F_n|_w}\sum_{\alpha\in F_n}d_\alpha\big\langle\pi_\varphi(\chi(\alpha))(\hat{1}), \hat{1}\big\rangle = \langle P(\hat{1}), \hat{1}\rangle.$$

Hence, $\lim_{n\to\infty}(1/|F_n|_w)\sum_{\alpha\in F_n}d_\alpha\varphi(\chi(\alpha)) \neq 0$ if and only if $P(\hat{1}) \neq 0$.

To prove $\lim_{n\to\infty}(1/|F_n|_w)\sum_{\alpha\in F_n}d_\alpha\varphi(\chi(\alpha)) = 0$ for $\varphi \neq \varepsilon$, it suffices to prove $P(\hat{1}) = 0$.

Suppose $P(\hat{1}) \neq 0$. Then $H_{\mathrm{inv}} \neq 0$. By Corollary 3.6, the space H_{inv} is an invariant subspace of $L^2(A, \varphi)$. Note that π_φ is irreducible since φ is a pure state. Hence $H_{\mathrm{inv}} = L^2(A, \varphi)$. In particular, $\hat{1} \in H_{\mathrm{inv}}$. Thus, for all $a \in A$, we have $\pi_\varphi(a)(\hat{1}) = \varepsilon(a)\hat{1}$. It follows that

$$\varphi(a) = \langle \pi_\varphi(a)(\hat{1}), \hat{1} \rangle = \langle \varepsilon(a)\hat{1}, \hat{1} \rangle = \varepsilon(a)$$

for all $a \in A$, which contradicts that $\varphi \neq \varepsilon$. □

4. A Wiener-type theorem for compact metrizable groups

In this section, we prove the following Wiener-type theorem:

Theorem 4.1. *Let G be a compact metrizable group. Given y in G and a right Følner sequence $\{F_n\}_{n=1}^{\infty}$ of $\widehat{G}$, for a finite Borel measure μ on G one has*

$$\lim_{n\to\infty} \frac{1}{|F_n|_w} \sum_{\alpha\in F_n} d_\alpha \sum_{1\le i,j\le d_\alpha} \mu(u_{ij}^\alpha)\overline{u_{ij}^\alpha(y)} = \mu\{y\} \quad \text{and} \quad \lim_{n\to\infty} \frac{1}{|F_n|_w} \sum_{\alpha\in F_n} d_\alpha \sum_{1\le i,j\le d_\alpha} |\mu(u_{ij}^\alpha)|^2 = \sum_{x\in G} \mu\{x\}^2.$$

Hence, μ is continuous if and only if

$$\lim_{n\to\infty} \frac{1}{|F_n|_w} \sum_{\alpha\in F_n} d_\alpha \sum_{1\le i,j\le d_\alpha} |\mu(u_{ij}^\alpha)|^2 = 0.$$

Here $(u_{ij}^\alpha)_{1\le i,j\le d_\alpha} \in M_{d_\alpha}(C(G))$ stands for a unitary matrix presenting $\alpha \in \widehat{G}$.

From now on G stands for a compact metrizable group. When thinking of G as a compact quantum group, the coproduct

$$\Delta : C(G) \to C(G) \otimes C(G)$$

is given by $\Delta(f)(x, y) = f(xy)$, the coinverse $\kappa : C(G) \to C(G)$ is given by $\kappa(f)(x) = f(x^{-1})$ and the counit $\varepsilon : C(G) \to \mathbb{C}$ is given by $\varepsilon(f) = f(e_G)$ for all $f \in C(G)$ and $x, y \in G$. Here, e_G is the neutral element of G.

Definition 4.2. Given a finite Borel measure μ on G, the *conjugate* $\bar{\mu}$ of μ is defined by

$$\bar{\mu}(f) = \int_G f(x^{-1})\, d\mu(x) = \mu(\kappa(f))$$

for all $f \in C(G)$, and $\bar{\mu}$ is also a finite Borel measure on G. In other words, $\bar{\mu}(E) = \mu(E^{-1})$ for every Borel subset E of G.

For $x \in G$, use δ_x to denote the Dirac measure at x.

The *convolution* $\mu * \nu$ of two finite Borel measures μ and ν on G is defined by

$$\mu * \nu(f) = (\mu \otimes \nu)\Delta(f) = \int_G \int_G f(xy)\, d\mu(x)\, d\nu(y)$$

for all $f \in C(G)$. For every Borel subset E of G, we have

$$\mu * \nu(E) = \int_G \nu(x^{-1}E)\, d\mu(x) = \int_G \mu(Ey^{-1})\, d\nu(y).$$

If either μ or ν is continuous, then so is $\mu * \nu$.

We can write a finite Borel measure μ on G as $\mu = \sum_i \lambda_i \delta_{x_i} + \mu_C$ for every atom x_i with $\mu\{x_i\} = \lambda_i$ and a finite continuous Borel measure μ_C.

Lemma 4.3. *Let μ be a finite Borel measure on G and $\{F_n\}_{n=1}^{\infty}$ be a right Følner sequence of $\widehat{G}$. Then*

$$\lim_{n\to\infty} \frac{1}{|F_n|_w} \sum_{\alpha\in F_n} d_\alpha \mu(\chi(\alpha)) = \mu\{e_G\}.$$

Proof. By Corollary 3.7, the sequence $\left\{(1/|F_n|_w) \sum_{\alpha\in F_n} d_\alpha \chi(\alpha)(x)\right\} \subseteq C(G)$ converges pointwise to 1_{e_G} (the characteristic function of $\{e_G\}$). The terms of the sequence are bounded by 1 for all $x \in G$; hence, by Lebesgue's dominated convergence theorem [Rudin 1987, Theorem 1.34], we have

$$\begin{aligned}\lim_{n\to\infty} \frac{1}{|F_n|_w} \sum_{\alpha\in F_n} d_\alpha \mu(\chi(\alpha)) &= \lim_{n\to\infty} \int_G \frac{1}{|F_n|_w} \sum_{\alpha\in F_n} d_\alpha \chi(\alpha)(x)\, d\mu(x)\\ &= \int_G \lim_{n\to\infty} \frac{1}{|F_n|_w} \sum_{\alpha\in F_n} d_\alpha \chi(\alpha)(x)\, d\mu(x)\\ &= \int_G 1_{e_G}\, d\mu = \mu\{e_G\}. \qquad \square\end{aligned}$$

Proof of Theorem 4.1. Given a finite Borel measure μ on G and $y \in G$, consider the measure $\mu * \delta_{y^{-1}}$. By Lemma 4.3, we have

$$\lim_{n\to\infty} \frac{1}{|F_n|_w} \sum_{\alpha\in F_n} d_\alpha \mu * \delta_{y^{-1}}(\chi(\alpha)) = \mu * \delta_{y^{-1}}\{e_G\}.$$

Note that

$$\begin{aligned}\mu * \delta_{y^{-1}}(\chi(\alpha)) &= \int_G \int_G \chi(\alpha)(xz)\, d\mu(x)\, d\delta_{y^{-1}}(z)\\ &= \int_G \chi(\alpha)(xy^{-1})\, d\mu(x)\\ &= \int_G \sum_{1\le i\le d_\alpha} u^\alpha_{ii}(xy^{-1})\, d\mu(x)\\ &= \int_G \sum_{1\le i\le d_\alpha} \sum_{1\le j\le d_\alpha} u^\alpha_{ij}(x) u^\alpha_{ji}(y^{-1})\, d\mu(x)\\ &= \int_G \sum_{1\le i\le d_\alpha} \sum_{1\le j\le d_\alpha} u^\alpha_{ij}(x) \overline{u^\alpha_{ij}(y)}\, d\mu(x).\end{aligned}$$

Moreover,

$$\mu * \delta_{y^{-1}}\{e_G\} = \int_G \int_G 1_{e_G}(xz)\, d\mu(x)\, d\delta_{y^{-1}}(z) = \int_G 1_{e_G}(xy^{-1})\, d\mu(x) = \mu\{y\}.$$

This completes the proof of the first part.

Applying Lemma 4.3 to $\mu * \bar{\mu}$, we have

$$\lim_{n\to\infty} \frac{1}{|F_n|_w} \sum_{\alpha\in F_n} d_\alpha \mu * \bar{\mu}(\chi(\alpha)) = \mu * \bar{\mu}\{e_G\}.$$

Since $\mu = \sum_{x_i \text{ atoms}} \lambda_i \delta_{x_i} + \mu_C$ with $\lambda_i = \mu\{x_i\}$ and μ_C a finite continuous Borel measure, we have

$$\bar{\mu} = \sum_{x_i \text{ atoms}} \lambda_i \bar{\delta}_{x_i} + \overline{\mu_C} = \sum_{x_i \text{ atoms}} \lambda_i \delta_{x_i^{-1}} + \overline{\mu_C}.$$

Hence,

$$\mu * \bar{\mu} = \sum_i \sum_j \lambda_i \lambda_j \delta_{x_i} * \delta_{x_j^{-1}} + \sum_i \lambda_i \delta_{x_i} * \overline{\mu_C} + \sum_j \lambda_j \mu_C * \delta_{x_j^{-1}} + \mu_C * \overline{\mu_C}.$$

Note that $\sum_i \lambda_i \delta_{x_i} * \overline{\mu_C} + \sum_j \lambda_j \mu_C * \delta_{x_j^{-1}} + \mu_C * \overline{\mu_C}$ is a finite continuous measure and

$$\sum_{i,j} \lambda_i \lambda_j \delta_{x_i} * \delta_{x_j^{-1}} = \sum_{i,j} \lambda_i \lambda_j \delta_{x_i x_j^{-1}}.$$

It follows that

$$\mu * \bar{\mu}\{e_G\} = \sum_{x_i \text{ atoms}} \lambda_i^2 = \sum_{x_i \text{ atoms}} \mu\{x_i\}^2 = \sum_{x\in G} \mu\{x\}^2.$$

On the other hand,

$$\begin{aligned}
\mu * \bar{\mu}(\chi(\alpha)) &= \int_G \int_G \chi(\alpha)(xy)\, d\mu(x)\, d\bar{\mu}(y) \\
&= \int_G \int_G \chi(\alpha)(xy^{-1})\, d\mu(x)\, d\mu(y) \\
&= \int_G \int_G \sum_{1\le i\le d_\alpha} u_{ii}^\alpha(xy^{-1})\, d\mu(x)\, d\mu(y) \\
&= \int_G \int_G \sum_{1\le i\le d_\alpha} \sum_{1\le j\le d_\alpha} u_{ij}^\alpha(x) u_{ji}^\alpha(y^{-1})\, d\mu(x)\, d\mu(y) \\
&= \sum_{1\le i\le d_\alpha} \sum_{1\le j\le d_\alpha} \int_G u_{ij}^\alpha(x)\, d\mu(x) \int_G \overline{u_{ij}^\alpha(y)}\, d\mu(y) \\
&= \sum_{1\le i,j\le d_\alpha} |\mu(u_{ij}^\alpha)|^2.
\end{aligned}$$

This ends the proof of the first part, and the second follows immediately. □

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References

[Anoussis and Bisbas 2000] M. Anoussis and A. Bisbas, "Continuous measures on compact Lie groups", *Ann. Inst. Fourier (Grenoble)* **50**:4 (2000), 1277–1296. MR 1799746 Zbl 0969.43001

[Bédos et al. 2001] E. Bédos, G. J. Murphy, and L. Tuset, "Co-amenability of compact quantum groups", *J. Geom. Phys.* **40**:2 (2001), 130–153. MR 1862084 Zbl 1011.46056

[Björklund and Fish 2009] M. Björklund and A. Fish, "Continuous measures on homogenous spaces", *Ann. Inst. Fourier (Grenoble)* **59**:6 (2009), 2169–2174. MR 2640917 Zbl 1194.60009

[Choi 1974] M. D. Choi, "A Schwarz inequality for positive linear maps on C^* -algebras", *Illinois J. Math.* **18**:4 (1974), 565–574. MR 0355615 Zbl 0293.46043

[Duvenhage 2008] R. Duvenhage, "A mean ergodic theorem for actions of amenable quantum groups", *Bull. Aust. Math. Soc.* **78**:1 (2008), 87–95. MR 2458300 Zbl 1160.46043

[Glasner 2003] E. Glasner, *Ergodic theory via joinings*, Mathematical Surveys and Monographs **101**, American Mathematical Society, Providence, RI, 2003. MR 1958753 Zbl 1038.37002

[Katznelson 2004] Y. Katznelson, *An introduction to harmonic analysis*, 3rd ed., Cambridge University Press, 2004. MR 2039503 Zbl 1055.43001

[Kyed 2008] D. Kyed, "L^2-Betti numbers of coamenable quantum groups", *Münster J. Math.* **1** (2008), 143–179. MR 2502497 Zbl 1195.46073

[Ruan 1996] Z.-J. Ruan, "Amenability of Hopf von Neumann algebras and Kac algebras", *J. Funct. Anal.* **139**:2 (1996), 466–499. MR 1402773 Zbl 0896.46041

[Rudin 1987] W. Rudin, *Real and complex analysis*, 3rd ed., McGraw-Hill, New York, 1987. MR 924157 Zbl 0925.00005

[Runde and Viselter 2014] V. Runde and A. Viselter, "Ergodic theory for quantum semigroups", *J. Lond. Math. Soc.* (2) **89**:3 (2014), 941–959. MR 3217657

[Taylor 1981] M. E. Taylor, *Pseudodifferential operators*, Princeton Mathematical Series **34**, Princeton University Press, 1981. MR 618463 Zbl 0453.47026

[Tomatsu 2006] R. Tomatsu, "A paving theorem for amenable discrete Kac algebras", *Internat. J. Math.* **17**:8 (2006), 905–919. MR 2261640 Zbl 1115.46057

[Wiener 1933] N. Wiener, *The Fourier integral and certain of its applications*, Dover, New York, 1933. MR 983891 Zbl 0006.05401

[Woronowicz 1987] S. L. Woronowicz, "Compact matrix pseudogroups", *Comm. Math. Phys.* **111** (1987), 613–665. MR 901157 Zbl 0627.58034

[Woronowicz 1998] S. L. Woronowicz, "Compact quantum groups", pp. 845–884 in *Symétries quantiques* (Les Houches, 1995), edited by A. Connes et al., North-Holland, Amsterdam, 1998. MR 1616348 Zbl 0997.46045

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RESONANCE FREE REGIONS FOR NONTRAPPING MANIFOLDS WITH CUSPS

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We prove resolvent estimates for nontrapping manifolds with cusps which imply the existence of arbitrarily wide resonance free strips, local smoothing for the Schrödinger equation, and resonant wave expansions. We obtain lossless limiting absorption and local smoothing estimates, but the estimates on the holomorphically continued resolvent exhibit losses. We prove that these estimates are optimal in certain respects.

1. Introduction

Resonance free regions near the essential spectrum have been extensively studied since the foundational work of Lax and Phillips and of Vaĭnberg. Their size is related to the dynamical structure of the set of trapped classical trajectories. More trapping typically results in a smaller region, and the largest resonance free regions exist when there is no trapping.

Example. Let $\mathbb{H}^2$ be the hyperbolic upper half plane. Let (X, g) be a nonpositively curved, compactly supported, smooth, metric perturbation of the quotient space $\langle z \mapsto z+1\rangle\backslash\mathbb{H}^2$. As we show in Section 2D, such a surface has no trapped geodesics (that is, all geodesics are unbounded).

Let (X, g) be as in the example above, or as in Section 2A, with dimension $n+1$ and Laplacian $\Delta \geq 0$. The resolvent $\left(\Delta - \frac{1}{4}n^2 - \sigma^2\right)^{-1}$ is holomorphic for $\operatorname{Im}\sigma > 0$, except at any $\sigma \in i\mathbb{R}$ such that $\sigma^2 + \frac{1}{4}n^2$ is an eigenvalue, and has essential spectrum $\{\operatorname{Im}\sigma = 0\}$; see Figure 1.

Theorem. *For all $\chi \in C_0^\infty(X)$, there exists $M_0 > 0$ such that for all $M_1 > 0$ there exists $M_2 > 0$ such that the cutoff resolvent $\chi\left(\Delta - \frac{1}{4}n^2 - \sigma^2\right)^{-1}\chi$ continues holomorphically to $\{|\operatorname{Re}\sigma| \geq M_2,\ \operatorname{Im}\sigma \geq -M_1\}$, where it obeys the estimate*

$$\left\|\chi\left(\Delta - \tfrac{1}{4}n^2 - \sigma^2\right)^{-1}\chi\right\|_{L^2(X)\to L^2(X)} \leq M_2|\sigma|^{-1+M_0|\operatorname{Im}\sigma|}. \tag{1-1}$$

In the example above, and in many of the examples in Section 2D, $\chi\left(\Delta - \frac{1}{4}n^2 - \sigma^2\right)^{-1}\chi$ is meromorphic in $\mathbb{C}$. The poles of the meromorphic continuation are called *resonances*.

Logarithmically large resonance free regions go back to work of Regge [1958] on potential scattering. In the setting of obstacle scattering they go back to work of Lax and Phillips [1989] and Vaĭnberg [1989], whose results were generalized by Morawetz, Ralston and Strauss [1977] and Melrose and Sjöstrand [1982]. When X is Euclidean outside of a compact set, they have been established for very general nontrapping perturbations of the Laplacian by Sjöstrand and Zworski in [2007, Theorem 1], which extends earlier work of Martinez [2002] and Sjöstrand [1990]. More recently, Baskin and Wunsch [2013],

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Keywords: cusp, resonances, resolvent, scattering, waves.

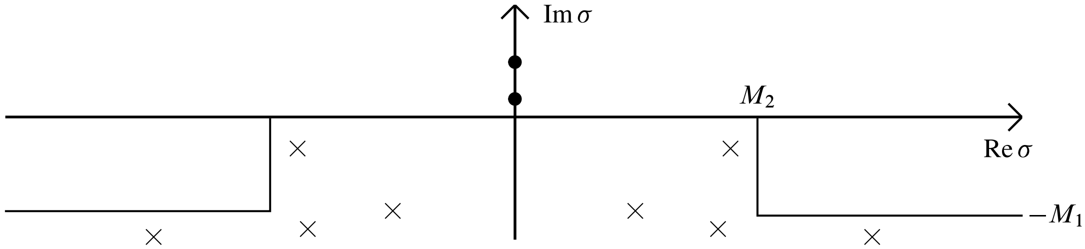

Figure 1. We prove that the cutoff resolvent continues holomorphically to arbitrarily wide strips and obeys polynomial bounds.

Galkowski and Smith [2015], and Galkowski [2015; 2016] have weakened slightly the sense in which the perturbation must be nontrapping. These works give a larger resonance free region and a stronger resolvent estimate than the Theorem above, but require asymptotically Euclidean geometry near infinity. On the other hand, as shown in recent work of Datchev, Kang and Kessler [2015], nontrapping manifolds with cusps which are merely $C^{1,1}$ (and not C^∞) do *not* have arbitrarily wide resonance free strips as in the Theorem.

The manifolds considered in this paper are nontrapping, but the cusp makes them not uniformly so: for a sufficiently large compact set $K \subset X$, we have

$$\sup_{\gamma\in\Gamma} \operatorname{diam} \gamma^{-1}(K) = +\infty,$$

where Γ is the set of unit-speed geodesics in X. This is because geodesics may travel arbitrarily far into the cusp before escaping down the funnel; this dynamical peculiarity makes it difficult to separate the analysis in the cusp from the analysis in the funnel and is the reason for the relatively involved resolvent estimate gluing procedure we use below.

Resonance free strips also exist in some trapping situations, with width determined by dynamical properties of the trapped set. These go back to work of Ikawa [1982], with recent progress by Nonnenmacher and Zworski [2009; 2015], Petkov and Stoyanov [2010], Alexandrova and Tamura [2011], Wunsch and Zworski [2011], Dyatlov [2015b], and Dyatlov and Zahl [2015]. Resonance free regions and resolvent estimates have applications to evolution equations, and this is an active area: examples include resonant wave expansions and wave decay, local smoothing estimates, Strichartz estimates, geometric control, wave damping, and radiation fields [Burq 2004; Burq and Zworski 2004; Bony and Häfner 2008; Guillarmou and Naud 2009; Christianson 2009; Burq, Guillarmou and Hassell 2010; Dyatlov 2012; 2015a; Melrose, Sá Barreto and Vasy 2014; Christianson, Schenck, Vasy and Wunsch 2014; Wang 2014]; see also [Wunsch 2012] for a recent survey and more references. In Section 7 we apply (1-1) to local smoothing and resonant wave expansions.

If (X, g) is evenly asymptotically hyperbolic (in the sense of Mazzeo and Melrose [1987] and Guillarmou [2005]) and nontrapping, then for any $M_1 > 0$ there is $M_2 > 0$ such that

$$\big\|\chi\big(\Delta - \tfrac{1}{4}n^2 - \sigma^2\big)^{-1}\chi\big\|_{L^2(X)\to L^2(X)} \le M_2|\sigma|^{-1}, \quad |\operatorname{Re}\sigma| \ge M_2,\ \operatorname{Im}\sigma \ge -M_1, \tag{1-2}$$

by work of Vasy [2013, (1.1)] (see also the analogous estimate for asymptotically Euclidean spaces by Sjöstrand and Zworski [2007, Theorem 1′], and related but slightly weaker estimates for more general asymptotically hyperbolic and conformally compact manifolds by Wang [2014] and Sá Barreto and Wang [2015]).

The bound (1-1) is weaker than (1-2) due to the presence of a cusp. Indeed, by studying low angular frequencies (which correspond to geodesics which travel far into the cusp before escaping down the funnel) in Proposition 8.1 we show that if $(X, g) = \langle z \mapsto z + 1\rangle \backslash \mathbb{H}^2$, then

$$\left\| \chi\left(\Delta - \tfrac{1}{4}n^2 - \sigma^2\right)^{-1} \chi \right\|_{L^2(X)\to L^2(X)} \geq e^{-C|\operatorname{Im}\sigma|} |\sigma|^{-1+2|\operatorname{Im}\sigma|}/C \tag{1-3}$$

for σ in the lower half-plane and near, but bounded away from, the real axis.

The lower bound (1-3) gives a sense in which (1-1) is optimal, but finding the maximal resonance free region remains an open problem. The only known explicit example of this type is $(X, g) = \langle z \mapsto z+1\rangle \backslash \mathbb{H}^2$, for which Borthwick [2007, §5.3] expresses the resolvent in terms of Bessel functions and shows there is only one resonance and it is simple (see also Proposition 8.1). On the other hand, Guillopé and Zworski [1997] study more general surfaces, and prove that if the 0-volume is not zero, then there are infinitely many resonances and optimal lower and upper bounds hold on their number in disks. We apply their result to our setting in Section 2D, giving a family of surfaces with infinitely many resonances to which our Theorem applies, but it is not clear even in this case whether or not the resonance free region given by the Theorem is optimal. The delicate nature of this question is indicated by the result in [Datchev, Kang and Kessler 2015] showing that nontrapping manifolds with cusps which are merely $C^{1,1}$ (and not C^∞) do *not* have arbitrarily wide resonance free strips.

Cardoso and Vodev [2002, Corollary 1.2], extending work of Burq [1998; 2002], proved resolvent estimates for very general infinite-volume manifolds (including the ones studied here; note that the presence of a funnel implies that the volume is infinite) which imply an exponentially small resonance free region. Our Theorem gives the first large resonance free region for a family of manifolds with cusps.

For $\operatorname{Im}\sigma = 0$, (1-1) is lossless; that is to say it agrees with the result for general nontrapping operators on asymptotically Euclidean or hyperbolic manifolds (see [Cardoso, Popov and Vodev 2004, (1.6)] and references therein). However, if (X, g) is asymptotically Euclidean or hyperbolic in the sense of [Datchev and Vasy 2012a, §4], then the gluing methods of that paper show that such a lossless estimate for $\operatorname{Im}\sigma = 0$ implies (1-2) for some $M_1 > 0$; see [Datchev 2012]. In this sense it is due to the cusp that $\mathcal{O}(|\sigma|^{-1})$ bounds hold for $\operatorname{Im}\sigma = 0$ but not in any strip containing the real axis.

The Theorem also provides a first step in support of the following:

Conjecture (fractal Weyl upper bound). *Let Γ be a geometrically finite discrete group of isometries of $\mathbb{H}^{n+1}$ such that $X = \Gamma\backslash\mathbb{H}^{n+1}$ is a smooth noncompact manifold. Let $R(X)$ denote the set of eigenvalues and resonances of X included according to multiplicity, let $K \subset T^*X$ be the set of maximally extended, bounded, unit speed geodesics, and let m be the Hausdorff dimension of K. Then for any $C_0 > 0$ there is $C_1 > 0$ such that, for $r \in \mathbb{R}$,*

$$\#\{\sigma \in R(X) : |\sigma - r| \leq C_0\} \leq C_1(1 + |r|)^{(m-1)/2}.$$

This statement is a partial generalization to the case of resonances of the Weyl asymptotic for eigenvalues of a compact manifold; such results go back to work of Sjöstrand [1990]. If $\Gamma\backslash\mathbb{H}^{n+1}$ has funnels but no cusps, this is proved in [Datchev and Dyatlov 2013] (generalizing earlier results of Zworski [1999] and Guillopé, Lin and Zworski [2004]); if $X=\Gamma\backslash\mathbb{H}^2$ has cusps but no funnels, this follows from work of Selberg [1990]. When $n=1$ the remaining case is $\Gamma\backslash\mathbb{H}^2$ having both cusps and funnels. The methods of the present paper, combined with those of [Sjöstrand and Zworski 2007; Datchev and Dyatlov 2013], provide a possible approach to the conjecture in this case. When $n\geq 2$, cusps can have mixed rank, and in this case even meromorphic continuation of the resolvent was proved only recently by Guillarmou and Mazzeo [2012].

In Section 2 we give the general assumptions on (X,g) under which the Theorem holds, and deduce consequences for the geodesic flow and for the spectrum of the Laplacian. We then give examples of manifolds which satisfy the assumptions, including examples with infinitely many resonances and examples with at least one eigenvalue.

In Section 3 we use a resolvent gluing method, based on one developed in [Datchev and Vasy 2012a], to reduce the Theorem to proving resolvent estimates and propagation of singularities results for three model operators. The first model operator is semiclassically elliptic outside of a compact set, and we analyze it in Section 4 following [Sjöstrand and Zworski 2007] and [Datchev and Vasy 2012a].

In Section 5 we study the second model operator, the model in the cusp. We use a separation of variables, a semiclassically singular rescaling, and an elliptic variant of the gluing method of Section 3 to reduce its study to that of a family of one-dimensional Schrödinger operators for which uniform resolvent estimates and propagation of singularities results hold. The rescaling causes losses for the resolvent estimate on the real axis, and we remove these by a noncompact variant of the method of propagation of singularities through trapped sets developed in [Datchev and Vasy 2012b]. The lower bound (1-3) shows that these losses cannot be removed for the continued resolvent; see also [Bony and Petkov 2013] for related and more general lower bounds in Euclidean scattering.

In Section 6 we study the third model operator, the model in the funnel, and we again reduce to a family of one-dimensional Schrödinger operators. To obtain uniform estimates we use a variant of the method of complex scaling of Aguilar and Combes [1971] and Simon [1972], following the geometric approach of Sjöstrand and Zworski [1991]. The method of complex scaling was first adapted to such families of operators by Zworski [1999], but we use here the approach of [Datchev 2010], which is slightly simpler and is adapted to nonanalytic manifolds. The analysis in this section could be replaced by that of [Vasy 2013], which avoids separating variables; the advantage of our approach is that it gives an estimate in a logarithmically large neighborhood of the real axis (although this does not make a difference here) and also requires less preliminary setup.

In Section 7 we apply (1-1) to local smoothing and resonant wave expansions. For the latter we need the additional assumption, satisfied in the example above and in many of the examples in Section 2D, that $\chi\big(\Delta-\frac{1}{4}n^2-\sigma^2\big)^{-1}\chi$ is meromorphic in $\mathbb{C}$. In Section 8 we prove (1-3) using Bessel function asymptotics.

2. Preliminaries

Throughout the paper $C > 0$ is a large constant which may change from line to line, and estimates are always uniform for $h \in (0, h_0]$, where $h_0 > 0$ may change from line to line.

2A. ***Assumptions.*** Let S be a compact manifold (without boundary) of dimension n, and let

$$X := \mathbb{R}_r \times S.$$

Let $R_g > 0$, and let g be a Riemannian metric on X such that

$$g|_{\{\pm r > R_g\}} = dr^2 + e^{2(r+\beta(r))} dS_\pm, \tag{2-1}$$

where dS_+ and dS_- are metrics on S, $R_g > 0$ and $\beta \in C^\infty(\mathbb{R})$. We call the region $\{r < -R_g\}$ the *cusp*, and the region $\{r > R_g\}$ the *funnel*; see Figure 2.

Suppose there is $\theta_0 \in \left(0, \frac{\pi}{4}\right)$ such that β is holomorphic and bounded in the sectors where $|z| > R_g$ and $\min\{|\arg z|, |\arg(-z)|\} < 2\theta_0$. By Cauchy estimates, for all $k \in \mathbb{N}$ there are $C, C_k > 0$, such that if $|z| > R_g$ and $\min\{|\arg z|,\ |\arg(-z)|\} \le \theta_0$, then

$$|\beta^{(k)}(z)| \le C_k |z|^{-k}, \ \ |\operatorname{Im} \beta(z)| \le C |\operatorname{Im} z|/|z|.$$

In particular, after possibly redefining R_g to be larger, we may assume without loss of generality that, for all $r \in \mathbb{R}$,

$$|\beta'(r)| + |\beta''(r)| \le \tfrac{1}{4}. \tag{2-2}$$

In the example at the beginning of the paper $\beta \equiv 0$. When the funnel end is an exact hyperbolic funnel, $\beta(r) = C + \log(1 + e^{-2r})$ for $r > R_g$.

We make two dynamical assumptions: if $\gamma : \mathbb{R} \to X$ is a maximally extended geodesic, assume $\gamma(\mathbb{R})$ is not bounded and $\gamma^{-1}(\{r < -R_g\})$ is connected. See Section 2D for examples.

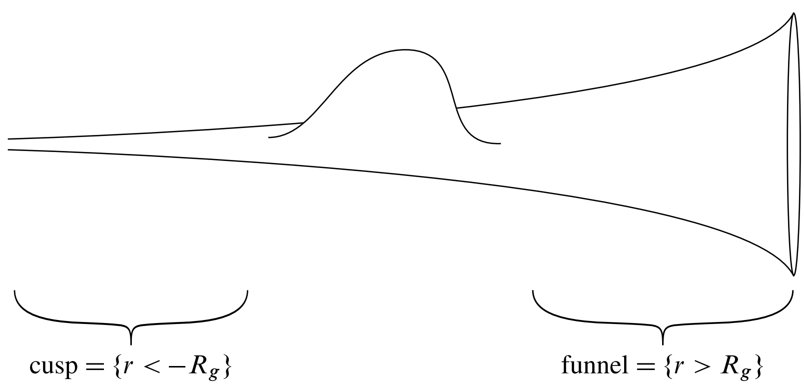

Figure 2. The manifold X.

2B. ***Dynamics near infinity.*** Let $p+1 \in C^\infty(T^*X)$ be the geodesic Hamiltonian; that is,

$$p = \rho^2 + e^{-2(r+\beta(r))}\sigma_\pm - 1$$

in the region $\{\pm r > R_g\}$, where ρ is dual to r, and $\sigma_\pm$ is the geodesic Hamiltonian of $(S, dS_\pm)$. From this we conclude that, along geodesic flow lines, we have

$$\dot r(t) = H_p\rho = 2\rho(t), \quad \dot\rho(t) = -H_p r = 2[1+\beta'(r(t))]e^{-2(r+\beta(r(t)))}\sigma_\pm,$$

so long as the trajectory remains within $\{\pm r > R_g\}$. In particular,

$$\ddot r(t) = 4[1+\beta'(r(t))]e^{-2(r+\beta(r(t)))}\sigma_\pm \ge 0. \tag{2-3}$$

Dividing the equation for $\dot\rho$ by $p+1-\rho^2$, putting $\hat\rho = \rho/\sqrt{p+1}$, and integrating we find

$$\tanh^{-1}\hat\rho(t) - \tanh^{-1}\hat\rho(0) = 2\sqrt{p+1}\left(t + \int_0^t \beta'(r(s))\,ds\right) \ge \frac{3}{4}\frac{r(t)-r(0)}{\max\{\hat\rho(s) : s \in [0,t]\}}, \tag{2-4}$$

where the equality holds so long as the trajectory remains in $\{\pm r > R_g\}$, and the inequality (which follows from (2-2) and the equation for $\dot r$) holds when additionally $t \ge 0$, $\rho(0) \ge 0$.

2C. ***The essential spectrum and semiclassical formulation of the problem.*** The nonnegative Laplacian is given by

$$\Delta|_{\{\pm r > R_g\}} = D_r^2 - in(1+\beta'(r))D_r + e^{-2(r+\beta(r))}\Delta_{S_\pm},$$

where $D_r = -i\partial_r$, and $\Delta_{S_\pm}$ is the Laplacian on $(S, dS_\pm)$. Fix $\varphi \in C^\infty(X)$ such that

$$\varphi|_{\{|r|>R_g\}} = \tfrac{1}{2}n(r+\beta(r)). \tag{2-5}$$

Then

$$(e^\varphi \Delta e^{-\varphi})\big|_{\{\pm r > R_g\}} = D_r^2 + e^{-2(r+\beta(r))}\Delta_{S_\pm} + \tfrac{1}{4}n^2 + V(r), \tag{2-6}$$

where

$$V(r) = \varphi'' + \varphi'^2 - \tfrac{1}{4}n^2 = \tfrac{1}{2}n\beta'' + \tfrac{1}{2}n^2\beta' + \tfrac{1}{4}n^2\beta'^2.$$

This shows that the essential spectrum of Δ is $\left[\frac{1}{4}n^2, \infty\right)$ (see for example [Reed and Simon 1978, Theorem XIII.14, Corollary 3]); the potential perturbation V is relatively compact since β' and β'' tend to zero at infinity (see for example Rellich's criterion [ibid., Theorem XIII.65]).

In this paper we study

$$P := h^2\left(e^\varphi \Delta e^{-\varphi} - \tfrac{1}{4}n^2\right) - 1. \tag{2-7}$$

This is an unbounded selfadjoint operator on $L^2_\varphi(X) := \{e^\varphi u : u \in L^2(X)\}$ with domain

$$H^2_\varphi(X) := \{u \in L^2_\varphi(X) : e^\varphi \Delta e^{-\varphi} u \in L^2_\varphi(X)\} = \{e^\varphi u : u \in H^2(X)\}.$$

Over the course of Sections 3–6 we will prove the following:

Proposition 2.1. *For every $\chi \in C_0^\infty(X)$, $E \in (0,1)$ there exists $C_0 > 0$ such that for every $\Gamma > 0$ there exist $C, h_0 > 0$ such that the cutoff resolvent $\chi(P-\lambda)^{-1}\chi$ continues holomorphically from $\{\operatorname{Im}\lambda > 0\}$ to $[-E, E] - i[0, \Gamma h]$ and satisfies*

$$\|\chi(P-\lambda)^{-1}\chi\|_{L^2_\varphi(X)\to L^2_\varphi(X)} \le C h^{-1-C_0|\operatorname{Im}\lambda|/h} \tag{2-8}$$

uniformly for $\lambda \in [-E, E] - i[0, \Gamma h]$ and $h \in (0, h_0]$.

This implies the Theorem.

2D. ***Examples.*** In this section we give a family of examples of manifolds satisfying the assumptions of Section 2A. I am very grateful to John Lott for suggesting this family of examples. In this section $d_g(p,q)$ denotes the distance between p and q with respect to the Riemannian metric g, and $L_g(c)$ denotes the length of a curve c with respect to g.

Let $(\mathbb{H}^{n+1}, g_h)$ be hyperbolic space with coordinates

$$(r, y) \in \mathbb{R} \times \mathbb{R}^n, \quad g_h := dr^2 + e^{2r} dy^2.$$

Let (X, g_h) be a parabolic cylinder obtained by quotienting the y variables to a torus:

$$X := \mathbb{R} \times \big(\langle y \mapsto y + c_1, \dots, y \mapsto y + c_n\rangle \backslash \mathbb{R}^n\big),$$

where the c_j are linearly independent vectors in $\mathbb{R}^n$. Let $R_g > 0$, put $dS_+ = dS_- = dy^2$, and take $\beta \in C^\infty(\mathbb{R})$ satisfying all assumptions of Section 2A, including (2-2). On $\{|r| > R_g\}$ define g by (2-1), and on $\{|r| \le R_g\}$ let g be any metric with all sectional curvatures nonpositive. The calculation in the Appendix shows that the sectional curvatures in $\{|r| > R_g\}$ are nonpositive so long as (2-2) holds.

The two dynamical assumptions in the last paragraph of Section 2A will follow from the following classical theorem (see for example [Bridson and Haefliger 1999, Theorem III.H.1.7]).

Proposition 2.2 (stability of quasigeodesics). *Let $(\mathbb{H}^{n+1}, g_h)$ be the $(n+1)$-dimensional hyperbolic space, let $p, q \in \mathbb{H}^{n+1}$, and let $\gamma_h : [t_1, t_2] \to \mathbb{H}^{n+1}$ be the unit-speed geodesic from p to q. Suppose $c : [t_1, t_2] \to \mathbb{H}^{n+1}$ satisfies $c(t_1) = p$, $c(t_2) = q$, and there is $C_1 > 0$ such that*

$$\frac{1}{C_1}|t - t'| \le d_{g_h}(c(t), c(t')) \le C_1|t - t'| \tag{2-9}$$

for all $t, t' \in [t_1, t_2]$. Then

$$\max_{t\in[t_1,t_2]} d_{g_h}(\gamma_h(t), c(t)) \le C_2, \tag{2-10}$$

where C_2 depends only on C_1.

To apply this theorem, observe first that just as g_h descends to a metric on X, so g lifts to a metric on $\mathbb{H}^{n+1}$; call the lifted metric g as well. Observe there is C_g such that

$$\frac{1}{C_g} g_h(u,u) \le g(u,u) \le C_g g_h(u,u), \quad u \in T_x X,\ x \in X. \tag{2-11}$$

Indeed, for x varying in a compact set this is true for any pair of metrics, and on $\{|r| > R_g\}$ it suffices if $C_g \ge e^{2\max|\beta|}$. We will show that if c is a unit-speed g-geodesic in $\mathbb{H}^n$, then (2-9) holds with a constant C_1 depending only on C_g. Since both g and g_h have nonnegative curvature and hence distance-minimizing geodesics, it is equivalent to show that

$$\frac{1}{C_1} d_g(p,q) \le d_{g_h}(p,q) \le C_1 d_g(p,q) \tag{2-12}$$

holds for all $p, q \in \mathbb{H}^{n+1}$, with a constant C_1 which depends only on C_g. For this last we compute as follows: let γ be a unit-speed g-geodesic from p to q. Then

$$d_{g_h}(p,q) \le L_{g_h}(\gamma) = \int_{t_1}^{t_2} \sqrt{g_h(\dot\gamma,\dot\gamma)}\, dt \le \int_{t_1}^{t_2} \sqrt{C_g g(\dot\gamma,\dot\gamma)}\, dt = \sqrt{C_g}\, L_g(\gamma) = \sqrt{C_g}\, d_g(p,q).$$

This proves the second inequality of (2-12), and the first follows from the same calculation since (2-11) is unchanged if we switch g and g_h.

Let $\gamma : \mathbb{R} \to X$ be a g-geodesic and $\gamma_h : \mathbb{R} \to X$ a g_h-geodesic. For any $x \in X$ we have

$$\lim_{t\to\infty} d_{g_h}(\gamma_h(t), x) = \lim_{t\to\infty} d_g(\gamma_h(t), x) = \infty,$$

and by (2-10) the same holds if γ_h is replaced by γ. In particular $\gamma(\mathbb{R})$ is not bounded.

We check finally that $\gamma^{-1}(\{r < -R_g\})$ is connected. It suffices to check that if instead $\gamma : \mathbb{R} \to \mathbb{H}^{n+1}$ is a g-geodesic, then $\gamma^{-1}(\{r < -N\})$ is connected for N large enough, with N independent of γ. We then conclude by redefining R_g to be larger than N.

We argue by way of contradiction. From (2-3) we see that $\dot r(t)$ is nondecreasing along γ in $\{r < -R_g\}$. Hence, if $\gamma^{-1}(\{r < -N\})$ is to contain at least two intervals for some $N > R_g$, there must exist times $t_1 < t_2 < t_3$ such that $r(\gamma(t_1)), r(\gamma(t_3)) < -N$ and $r(\gamma(t_2)) = -R_g$. Now the g_h-geodesic $\gamma_h : [t_1, t_3] \to \mathbb{H}^n$ joining $\gamma(t_1)$ to $\gamma(t_3)$ has $r(\gamma_h(t)) < -N$ for all $t \in [t_1, t_3]$. It follows that $d_{g_h}(\gamma_h(t_2), \gamma(t_2)) \ge N - R_g$, and if N is large enough this violates (2-10).

2D1. *Examples with infinitely many resonances.* In this subsection we specialize to the case $n = 1$, $\beta(r) = 0$ for $r < -R_g$, $\beta(r) = \beta_0 + \log(1 + e^{-2r})$ for $r > R_g$ and for some $\beta_0 \in \mathbb{R}$. Then the cusp and funnel of X are isometric to the standard cusp and funnel obtained by quotienting $\mathbb{H}^2$ by a *nonelementary* Fuchsian subgroup (see, e.g., [Borthwick 2007, §2.4]; note that the funnel end is slightly different here than in the example at the beginning of the paper).

In particular there is $l > 0$ such that

$$X = \mathbb{R}_r \times (\mathbb{R}/l\mathbb{Z})_t, \quad g|_{\{r > R_g\}} = dr^2 + \cosh^2 r\, dt^2.$$

If $(X_0, g_0) = [0,\infty) \times (\mathbb{R}/l\mathbb{Z})$, $g_0 = dr^2 + \cosh^2 r\, dt^2$, then the 0-volume of X is

$$\text{0-vol}(X) \stackrel{\text{def}}{=} \operatorname{vol}_g(X \cap \{r < R_g\}) - \operatorname{vol}_{g_0}(X_0 \cap \{r < R_g\}).$$

Let $R_\chi(\sigma)$ denote the meromorphic continuation of $\chi\big(\Delta - \frac{1}{4} - \sigma^2\big)^{-1}\chi$. In this case, $R_\chi(\sigma)$ is meromorphic in $\mathbb{C}$ [Mazzeo and Melrose 1987; Guillopé and Zworski 1997], and near each pole σ_0 we have

$$R_\chi(\sigma) = \chi\left(\sum_{j=1}^{k} \frac{A_j}{(\sigma-\sigma_0)^j} + A(\sigma)\right)\chi,$$

where the $A_j : L^2_{\mathrm{comp}}(X) \to L^2_{\mathrm{loc}}(X)$ are finite rank and $A(\sigma)$ is holomorphic near σ_0. The *multiplicity* of a pole, $m(\sigma_0)$ is given by

$$m(\sigma) \stackrel{\mathrm{def}}{=} \operatorname{rank}\left(\sum_{j=1}^{k} A_j\right).$$

Proposition 2.3 [Guillopé and Zworski 1997, Theorem 1.3]. *If* 0-vol$(X) \neq 0$, *then there exists a constant C such that*

$$\lambda^2/C \le \sum_{|\sigma|\le\lambda} m(\sigma) \le C\lambda^2, \quad \lambda > C.$$

We can ensure that 0-vol$(X) \neq 0$ by adding, if necessary, a small compactly supported metric perturbation to g. Then, as $\lambda \to \infty$, the meromorphic continuation of R_χ will have $\sim \lambda^2$-many poles in a disk of radius λ, but none of them will be in the strips (1-1).

2D2. *Examples with at least one eigenvalue.* In this subsection we consider examples of the form

$$X := \mathbb{R} \times (\mathbb{R}^n/\mathbb{Z}^n), \quad g := dr^2 + \exp\left(2r + 2\int_{-\infty}^{r} b\right) dy^2, \quad b \in C_0^\infty(\mathbb{R}). \tag{2-13}$$

As in (2-3), we have $\ddot{r} = 4(1+b(r))e^{-2(r+\int^r b)}\sigma$, and this is nonnegative as long as $b \ge -1$; consequently, as long as $b \ge -1$ the assumptions of Section 2A hold. We will give a sufficient condition on b such that X has at least one eigenvalue, and also infinitely many resonances.

By the calculation in Section 2C, if $\varphi(r) := \frac{1}{2}\big(r + \int_{-\infty}^{r} b\big)$ for all $r \in \mathbb{R}$, then

$$e^{-\varphi}\Delta e^{\varphi} = D_r^2 + e^{-2(r+\int^r b)}\Delta_{\mathbb{R}^n/\mathbb{Z}^n} + \tfrac{1}{4}n^2 + V(r), \quad V(r) := \tfrac{1}{2}nb'(r) + \tfrac{1}{4}n^2 b(r)^2 + \tfrac{1}{2}n^2 b(r).$$

Note $V \in C_0^\infty(\mathbb{R})$, and consequently (see for example [Reed and Simon 1978, Theorem XIII.110]) $D_r^2 + V(r)$ has a negative eigenvalue provided $V \not\equiv 0$ and $\int V \le 0$; it suffices for example to take $b \le 0$. But Zworski [1987, Theorem 2] has shown that if $V \not\equiv 0$, then $D_r^2 + V(r)$ has infinitely many resonances: indeed, the number in a disk of radius λ is given by

$$\frac{2}{\pi}(\operatorname{diam}\operatorname{supp} V)\lambda + o(\lambda), \quad \lambda \to \infty.$$

This eigenvalue and these resonances correspond to an eigenvalue and resonances for Δ: one multiplies the eigenfunction and resonant states by e^{φ} and regards them as functions on X which depend on r only.

In summary, if (X, g) is given by (2-13), then the assumptions of Section 2A hold if $b \ge -1$. It has infinitely many resonances and at least one eigenvalue if additionally $b \not\equiv 0$, $b \le 0$.

2E. *Pseudodifferential operators.* In this section we review some facts about semiclassical pseudodifferential operators, following [Dimassi and Sjöstrand 1999; Zworski 2012; Dyatlov and Zworski 2016].

2E1. *Pseudodifferential operators on* $\mathbb{R}^n$. For $m \in \mathbb{R}$, $\delta \in \left[0, \frac{1}{2}\right)$, let $S^m_\delta(\mathbb{R}^n)$ be the symbol class of functions $a = a_h(x, \xi) \in C^\infty(T^*\mathbb{R}^n)$ satisfying

$$|\partial_x^\alpha \partial_\xi^\beta a| \le C_{\alpha,\beta} h^{-\delta(|\alpha|+|\beta|)} (1 + |\xi|^2)^{(m-|\beta|)/2} \tag{2-14}$$

uniformly in $T^*\mathbb{R}^n$. The *principal symbol* of a is its equivalence class in $S^m_\delta(\mathbb{R}^n)/hS^{m-1}_\delta(\mathbb{R}^n)$. Let $S^m(\mathbb{R}^n) = S^m_0(\mathbb{R}^n)$.

We quantize $a \in S^m_\delta(\mathbb{R}^n)$ to an operator $\mathrm{Op}(a)$ using the formula

$$(\mathrm{Op}(a)u)(x) = \frac{1}{(2\pi h)^n} \iint e^{i(x-y)\cdot\xi/h} a_h(x, \xi) u(y)\, dy\, d\xi, \tag{2-15}$$

and put $\Psi^m_\delta(\mathbb{R}^n) = \{\mathrm{Op}(a) : a \in S^m_\delta(\mathbb{R}^n)\}$, $\Psi^m(\mathbb{R}^n) = \Psi^m_0(\mathbb{R}^n)$. If $A = \mathrm{Op}(a)$ then a is the *full symbol* of A, and the principal symbol of A is the principal symbol of a. If $A \in \Psi^m_\delta(\mathbb{R}^n)$, then for any $s \in \mathbb{R}$ we have $\|A\|_{H_h^{s+m}(\mathbb{R}^n) \to H_h^s(\mathbb{R}^n)} \le C$, where (if $\Delta \ge 0$)

$$\|u\|_{H_h^s(\mathbb{R}^n)} = \|(1 + h^2\Delta)^{s/2} u\|_{L^2(\mathbb{R}^n)}.$$

If $A \in \Psi^m_\delta(\mathbb{R}^n)$ and $B \in \Psi^{m'}_\delta(\mathbb{R}^n)$, then $AB \in \Psi^{m+m'}_\delta(\mathbb{R}^n)$ and $[A, B] = AB - BA \in h^{1-2\delta}\Psi^{m+m'-1}_\delta(\mathbb{R}^n)$. If a and b are the principal symbols of A and B, then the principal symbol of $h^{2\delta-1}[A, B]$ is $iH_b a$, where H_b is the Hamiltonian vector field of b.

If $K \subset T^*\mathbb{R}^n$ has either K or $T^*\mathbb{R}^n \setminus K$ bounded in ξ, then $a \in S^m_\delta(\mathbb{R}^n)$ is *elliptic* on K if

$$|a| \ge (1 + |\xi|^2)^{m/2}/C \tag{2-16}$$

uniformly for $(x, \xi) \in K$. We say that $A \in \Psi^m_\delta(\mathbb{R}^n)$ is elliptic on K if its principal symbol is. For such K, we say A is *microsupported* in K if the full symbol a of A obeys

$$|\partial_x^\alpha \partial_\xi^\beta a| \le C_{\alpha,\beta,N} h^N (1 + |\xi|^2)^{-N} \tag{2-17}$$

uniformly on $T^*\mathbb{R}^n \setminus K$, for any α, β, N. If A_1 is microsupported in K_1 and A_2 is microsupported in K_2, then $A_1 A_2$ is microsupported in $K_1 \cap K_2$.

If $A \in \Psi^m_\delta(\mathbb{R}^n)$ is elliptic on K, then it is invertible there in the following sense: there exists $G \in \Psi^{-m}_\delta(\mathbb{R}^n)$ such that $AG - \mathrm{Id}$ and $GA - \mathrm{Id}$ are both microsupported in $T^*\mathbb{R}^n \setminus K$. Hence if $B \in \Psi^{m'}_\delta(\mathbb{R}^n)$ is microsupported in K and A is elliptic in an ε-neighborhood of K for some $\varepsilon > 0$, then, for any $s, N \in \mathbb{R}$,

$$\|Bu\|_{H_h^{s+m}(\mathbb{R}^n)} \le C\|ABu\|_{H_h^s(\mathbb{R}^n)} + \mathcal{O}(h^\infty)\|u\|_{H_h^{-N}(\mathbb{R}^n)}. \tag{2-18}$$

The *sharp Gårding inequality* says that if the principal symbol of $A \in \Psi^m_\delta(\mathbb{R}^n)$ is nonnegative near K and $B \in \Psi^{m'}_\delta(\mathbb{R}^n)$ is microsupported in K, then

$$\langle ABu, Bu\rangle_{L^2(\mathbb{R}^n)} \ge -Ch^{1-2\delta}\|Bu\|^2_{H^{(m-1)/2}(\mathbb{R}^n)} - \mathcal{O}(h^\infty)\|u\|_{H_h^{-N}(\mathbb{R}^n)}. \tag{2-19}$$

2E2. *Pseudodifferential operators on a manifold.* These results extend to the case of a noncompact manifold X, provided we require our estimates to be uniform only on compact subsets of X. For convenience we work in the setting of Section 2A, with the notation of Section 2C, but the discussion below applies to any manifold; see also the discussions in [Datchev and Dyatlov 2013, §3.1] and [Dyatlov and Zworski 2016, Appendix E]. Note that we take care to quantize a symbol which is compactly supported in space to an operator which is compactly supported in space.

Write $S^m_\delta(X)$ for the symbol class of functions $a \in C^\infty(T^*X)$ satisfying (2-14) on coordinate patches (note that this condition is invariant under change of coordinates). The principal symbol of a is its equivalence class in $S^m_\delta(X)/hS^{m-1}_\delta(X)$, and let $S^m(X) = S^m_0(X)$.

Let $h^\infty\Psi^{-\infty}(X)$ be the set of linear operators R such that for any $\chi \in C^\infty_0(X)$, we have

$$\|\chi R\|_{H^{-N}_{\varphi,h}(X)\to H^N_{\varphi,h}(X)} + \|R\chi\|_{H^{-N}_{\varphi,h}(X)\to H^N_{\varphi,h}(X)} \le C_N h^N$$

for any N, where

$$\|u\|_{H^s_{\varphi,h}(X)} := \|(2+P)^{s/2}u\|_{L^2_\varphi(X)}. \tag{2-20}$$

We quantize $a \in S^m_\delta(X)$ to an operator $\mathrm{Op}(a)$ by using a partition of unity and the formula (2-15) in coordinate patches. Let $\Psi^m_\delta(X) = \{\mathrm{Op}(a) + R : a \in S^m_\delta(X),\ R \in h^\infty\Psi^{-\infty}(X)\}$. The quantization Op depends on the choices of coordinates and partition of unity, but the class $\Psi^m_\delta(X)$ does not. If $A \in \Psi^m_\delta(X)$ and $\chi \in C^\infty_0(X)$, then χA and $A\chi$ are bounded as operators $H^{s+m}_{\varphi,h}(X) \to H^s_{\varphi,h}(X)$, uniformly in h. If $A \in \Psi^m_\delta(X)$ and $B \in \Psi^{m'}_\delta(X)$, then

$$AB \in \Psi^{m+m'}_\delta(X) \quad \text{and} \quad h^{2\delta-1}[A,B] \in \Psi^{m+m'-1}_\delta(X).$$

If a and b are the principal symbols of A and B (the principal symbol is invariantly defined, although the total symbol is not), then the principal symbol of $h^{2\delta-1}[A,B]$ is $iH_b a$, where H_b is the Hamiltonian vector field of b.

Let $K \subset T^*X$ have either $K \cap T^*U$ bounded for every bounded $U \subset X$, or $T^*U \setminus K$ bounded for every bounded $U \subset X$. We say $a \in S^m_\delta(X)$ is *elliptic* on K if (2-16) holds uniformly on $T^*U \cap K$ for every bounded $U \subset X$. We say that $A \in \Psi^m_\delta(X)$ is elliptic on K if its principal symbol is. We say A is *microsupported* in K if a full symbol a of A obeys (2-17) uniformly on $T^*U \setminus K$ for every bounded $U \subset X$ and for any α, β, N (note that if this holds for one full symbol of A, it also does for all the others).

If $B \in \Psi^{m'}_\delta(X)$ is microsupported in K and A is elliptic in an ε-neighborhood of K for some $\varepsilon > 0$, then, for any $s, N \in \mathbb{R}$ and $\chi \in C^\infty_0(X)$,

$$\|B\chi u\|_{H^{s+m}_{\varphi,h}(X)} \le C\|AB\chi u\|_{H^s_{\varphi,h}(X)} + \mathcal{O}(h^\infty)\|\chi u\|_{H^{-N}_{\varphi,h}(X)}. \tag{2-21}$$

The *sharp Gårding inequality* says that if the principal symbol of $A \in \Psi^m_\delta(X)$ is nonnegative near K and $B \in \Psi^{m'}_\delta(X)$ is microsupported in K, then for every $\chi \in C^\infty_0(X)$, $N \in \mathbb{R}$,

$$\langle AB\chi u, B\chi u\rangle_{L^2_\varphi(X)} \ge -Ch^{1-2\delta}\|B\chi u\|^2_{H^{(m-1)/2}_{\varphi,h}(X)} - \mathcal{O}(h^\infty)\|\chi u\|_{H^{-N}_{\varphi,h}(X)}. \tag{2-22}$$

2E3. *Exponentiation of operators.* For $q \in C_0^\infty(T^*X)$, $Q = \mathrm{Op}(q)$, and $\varepsilon \in [0, C_0 h \log(1/h)]$, we will be interested in operators of the form $e^{\varepsilon Q/h}$. By the discussion above, since $q \in S^m(X)$ for every $m \in \mathbb{R}$, we have $\|Q\|_{H^{-N}_{\varphi,h} \to H^N_{\varphi,h}} \le C_N$ for every $N \in \mathbb{R}$.

We write

$$e^{\varepsilon Q/h} := \sum_{j=0}^{\infty} \frac{(\varepsilon/h)^j}{j!} Q^j,$$

with the sum converging in the $H^s_{\varphi,h}(X) \to H^s_{\varphi,h}(X)$ norm operator topology, but the convergence is not uniform as $h \to 0$. Beals's characterization [Zworski 2012, Theorem 9.12] can be used to show that $e^{\varepsilon Q/h} \in \Psi^0_\delta(X)$ for any $\delta > 0$, but we will not need this. Let $s \in \mathbb{R}$. Then

$$\|e^{\varepsilon Q/h}\| \le \sum_{j=0}^{\infty} \frac{(C_0 \log(1/h))^j}{j!} \|Q\|^j = e^{C_0 \log(1/h)\|Q\|} = h^{-C_0\|Q\|}, \tag{2-23}$$

where all norms are $H^s_{\varphi,h}(X) \to H^s_{\varphi,h}(X)$.

If $A \in \Psi^m_\delta(X)$ is bounded as an operator $H^{s+m}_{\varphi,h}(X) \to H^s_{\varphi,h}(X)$, uniformly in h, (without needing to be multiplied by a cutoff), then, by (2-23),

$$\|e^{\varepsilon Q/h} A e^{-\varepsilon Q/h}\|_{H^{s+m}_{\varphi,h}(X) \to H^s_{\varphi,h}(X)} \le C h^{-N} \tag{2-24}$$

for any $s \in \mathbb{R}$, where

$$N = C_0(\|Q\|_{H^{s+m}_{\varphi,h}(X) \to H^{s+m}_{\varphi,h}(X)} + \|Q\|_{H^s_{\varphi,h}(X) \to H^s_{\varphi,h}(X)}).$$

But, writing $\mathrm{ad}_Q A = [Q, A]$ and $e^{\varepsilon Q/h} A e^{-\varepsilon Q/h} = e^{\varepsilon\, \mathrm{ad}_Q/h} A$, for any $J \in \mathbb{N}$ we have the Taylor expansion

$$e^{\varepsilon Q/h} A e^{-\varepsilon Q/h} = \sum_{j=0}^{J} \frac{\varepsilon^j}{j!} \left(\frac{\mathrm{ad}_Q}{h}\right)^j A + \frac{\varepsilon^{J+1}}{J!} \int_0^1 (1-t)^J e^{-\varepsilon t\, \mathrm{ad}_Q/h} \left(\frac{\mathrm{ad}_Q}{h}\right)^{J+1} A\, dt. \tag{2-25}$$

For any $M \in \mathbb{N}$, the integrand maps $H^M_{\varphi,h}(X)$ to $H^{-M}_{\varphi,h}(X)$ with norm $\mathcal{O}(h^{-2\delta(J+1)-N})$, where

$$N = C_0(\|Q\|_{H^M_{\varphi,h}(X) \to H^M_{\varphi,h}(X)} + \|Q\|_{H^{-M}_{\varphi,h}(X) \to H^{-M}_{\varphi,h}(X)}).$$

Hence applying (2-25) with J sufficiently large we see that (2-24) can be improved to

$$\|e^{\varepsilon Q/h} A e^{-\varepsilon Q/h}\|_{H^{s+m}_{\varphi,h}(X) \to H^s_{\varphi,h}(X)} \le C,$$

and the integrand in (2-25) maps $H^M_{\varphi,h}(X)$ to $H^{-M}_{\varphi,h}(X)$ with norm $\mathcal{O}(1)$. Applying (2-25) with $J \to \infty$ shows that $e^{\varepsilon Q/h} A e^{-\varepsilon Q/h} \in \Psi^m_\delta(X)$, and applying (2-25) with $J = 1$ we find

$$e^{\varepsilon Q/h} A e^{-\varepsilon Q/h} = A - \varepsilon[A, Q/h] + \varepsilon^2 h^{-4\delta} R, \tag{2-26}$$

where $R \in \Psi^{-\infty}_\delta(X)$.

3. Reduction to estimates for model operators

3A. ***Resolvent gluing.*** In Section 2 we showed that the Theorem follows from (2-8). In this section, we reduce (2-8) to several estimates for model operators using a variant of the gluing method of [Datchev and Vasy 2012a], adapted to the dynamics on X.

We will use the following open cover of X:

$$\Omega_C := \{r < -R_g\}, \quad \Omega_K := \{|r| < R_g + 3\}, \quad \Omega_F := \{r > R_g\}.$$

Let P_C, P_K, P_F be differential operators on X which are *model operators* for P, with respect to this open cover, in the sense that they satisfy

$$P_j|_{\Omega_j} = P|_{\Omega_j}, \quad j \in \{C, K, F\}. \tag{3-1}$$

So P_C is a model in the cusp, P_F is a model in the funnel, and P_K is a model in a neighborhood of the remaining region (see Figure 2).

More specifically, let $W_K \in C^\infty(X; [0, 1])$ be 0 near $\{|r| \le R_g + 3\}$, and 1 near $\{|r| \ge R_g + 4\}$, and let

$$P_K = P - i W_K;$$

let $W_C \in C^\infty(\mathbb{R}; [0, 1])$ be 0 near $\{r \le -R_g\}$, and 1 near $\{r \ge 0\}$, and let

$$P_C = h^2 D_r^2 + h^2 e^{-2(r+\beta(r))} \Delta_{S_-} + h^2 V(r) - 1 - i W_C(r);$$

let $W_F \in C^\infty(\mathbb{R}; [0, 1])$ be 0 near $\{r \ge R_g\}$, and 1 near $\{r \le 0\}$, nonincreasing, and let

$$P_F = h^2 D_r^2 + h^2 (1 - W_F(r)) e^{-2(r+\beta(r))} \Delta_{S_+} + h^2 V(r) - 1 - i W_F(r).$$

The functions W_j for $j \in \{C, K, F\}$, are called *complex absorbing barriers* and they make each P_j semiclassically elliptic in the region where $W_j = 1$. Note that we have also chosen P_C and P_F so that we can separate variables, and so that P_F has no exponentially growing term.

Now observe that $P_j + i W_j$ is selfadjoint on L^2_j, where

$$L^2_K := L^2_\varphi(X), \quad L^2_C := L^2(X, dr\, dS_-), \quad L^2_F := L^2(X, dr\, dS_+).$$

Moreover, $W_j \ge 0$ implies $\langle \operatorname{Im} P_j u, u\rangle_{L^2_j} \le 0$, and hence

$$\|u\|_{L^2_j} \le (\operatorname{Im}\lambda)^{-1} \|(P_j - \lambda)u\|_{L^2_j}, \quad \operatorname{Im}\lambda > 0,$$

and, consequently (since W_j is bounded on L^2_j), when $\operatorname{Im}\lambda > 0$, we can define the resolvents

$$R_j(\lambda) := (P_j - \lambda)^{-1} : L^2_j \to L^2_j, \quad j \in \{C, K, F\}.$$

Using (2-20) and (3-1) gives, for any $\chi_j \in C^\infty(X)$, bounded with all derivatives, and satisfying $\operatorname{supp} \chi_j \subset \Omega_j$,

$$\max_{j \in \{C,K,F\}} \|\chi_j R_j(\lambda) \chi_j\|_{L^2_\varphi(X) \to H^2_{\varphi,h}(X)} \le C(|\lambda| + (\operatorname{Im}\lambda)^{-1}), \quad \operatorname{Im}\lambda > 0. \tag{3-2}$$

Below we will show that for every $\chi_j \in C_0^\infty(X)$ with $\operatorname{supp}\chi_j \subset \Omega_j$, $E \in (0,1)$, there is $C_0 > 0$ such that for all $\Gamma > 0$ the cutoff resolvents $\chi_j R_j(\lambda)\chi_j$ continue holomorphically to $\lambda \in [-E, E] + i[-\Gamma h, \infty)$, where they satisfy

$$\max_{j\in\{C,K,F\}} \|\chi_j R_j(\lambda)\chi_j\|_{L^2_\varphi(X)\to H^2_{\varphi,h}(X)} \le C h^{-1-C_0|\operatorname{Im}\lambda|/5h}. \tag{3-3}$$

Here E, C_0, and Γ are the same as in (2-8), but as elsewhere in the paper the constant C and the implicit constant h_0 may be different.

We will also show that the $R_j(\lambda)$ propagate singularities forward along bicharacteristics, in the following limited sense. Let $\chi_1 \in C_0^\infty(X)$ and let $\chi_2, \chi_3 \in \Psi^1(X)$ be compactly supported differential operators.

- Suppose $\operatorname{supp}\chi_1 \subset \Omega_K$, $\operatorname{supp}\chi_2 \subset \Omega_K \cap \Omega_F$, and $\operatorname{supp}\chi_3 \subset \Omega_F$. If further $\operatorname{supp}\chi_1 \cup \operatorname{supp}\chi_3 \subset \{r < R_g + 2\}$ and $\operatorname{supp}\chi_2 \subset \{r > R_g + 2\}$, then, for any $N \in \mathbb{N}$,

$$\|\chi_3 R_F(\lambda)\chi_2 R_K(\lambda)\chi_1\|_{L^2_\varphi(X)\to L^2_\varphi(X)} = \mathcal{O}(h^\infty) \tag{3-4}$$

  uniformly for $|\operatorname{Re}\lambda| \le E$, $\operatorname{Im}\lambda \in [-\Gamma h, h^{-N}]$.

- Suppose $\operatorname{supp}\chi_1 \subset \Omega_C$, $\operatorname{supp}\chi_2 \subset \Omega_C \cap \Omega_K$, and $\operatorname{supp}\chi_3 \subset \Omega_K$. If further $\operatorname{supp}\chi_1 \cup \operatorname{supp}\chi_3 \subset \{r < -R_g - 2\}$ and $\operatorname{supp}\chi_2 \subset \{r > -R_g - 2\}$, then, for any $N \in \mathbb{N}$,

$$\|\chi_3 R_K(\lambda)\chi_2 R_C(\lambda)\chi_1\|_{L^2_\varphi(X)\to L^2_\varphi(X)} = \mathcal{O}(h^\infty) \tag{3-5}$$

  uniformly for $|\operatorname{Re}\lambda| \le E$, $\operatorname{Im}\lambda \in [-\Gamma h, h^{-N}]$.

Note that in either case there can exist no bicharacteristic passing through $T^*\operatorname{supp}\chi_1$, $T^*\operatorname{supp}\chi_2$, $T^*\operatorname{supp}\chi_3$ in that order. In the first case this is implied by (2-3), and in the second by (2-3) together with the assumption that $\gamma^{-1}(\{r < -R_g\})$ is connected for any geodesic $\gamma : \mathbb{R} \to X$. We will use these facts in the proofs of (3-4) and (3-5) below. Before doing that, however, we will show that these estimates imply the Theorem.

Proposition 3.1. *The estimate* (2-8) *follows from* (3-3), (3-4), *and* (3-5).

Proof. Let $\chi_C, \chi_K, \chi_F \in C^\infty(\mathbb{R})$ satisfy $\chi_C + \chi_K + \chi_F = 1$, $\operatorname{supp}\chi_F \subset (R_g + 1, \infty)$, $\operatorname{supp}(1 - \chi_F) \subset (R_g + 2, \infty)$, and $\chi_C(r) = \chi_F(-r)$ for all $r \in \mathbb{R}$. Then define a parametrix for $P - \lambda$ by

$$G = \chi_C(r-1)R_C(\lambda)\chi_C(r) + \chi_K(|r-1|)R_K(\lambda)\chi_K(|r|) + \chi_F(r+1)R_F(\lambda)\chi_F(r).$$

Then G is defined for $\operatorname{Im}\lambda > 0$ and $\chi G\chi$ continues holomorphically to $\lambda \in [-E, E] - i[0, \Gamma h]$. Define operators A_C, A_K, A_F by

$$\begin{aligned}(P-\lambda)G &= \operatorname{Id} + [\chi_C(r-1), h^2D_r^2]R_C(\lambda)\chi_C(r) + [\chi_K(|r-1|), h^2D_r^2]R_K(\lambda)\chi_K(|r|)\\ &\qquad + [\chi_F(r+1), h^2D_r^2]R_F(\lambda)\chi_F(r)\\ &= \operatorname{Id} + A_C + A_K + A_F;\end{aligned}$$

Figure 3. The remainders A_C, A_K, and A_F are localized on the right in the region to the back of the arrows, and on the left near the tips of the arrows (A_C is localized on the right at the support of χ_C and on the left at the support of $\chi'_C(\cdot - 1)$, and so on), and this implies (3-6). They are microlocalized on the left in the indicated directions, and this implies (3-7) (since, by (2-3), no geodesic can follow one of the A_K arrows and then the A_F arrow, and so on).

see Figure 3. The estimates (3-2) and (3-3) only allow us to remove the remainders A_C, A_K, A_F by Neumann series for a narrow range of λ. To obtain a parametrix with improved remainders, observe that the support properties of the χ_j imply that

$$A_C^2 = A_K^2 = A_F^2 = A_C A_F = A_F A_C = 0; \tag{3-6}$$

so, solving away using G, we obtain

$$(P-\lambda)G(\mathrm{Id} - A_C - A_K - A_F) = \mathrm{Id} - A_K A_C - A_C A_K - A_F A_K - A_K A_F.$$

Now the propagation of singularities estimates (3-4) and (3-5) imply

$$\|A_F A_K\|_{L^2_\varphi(X)\to L^2_\varphi(X)} + \|A_C A_K A_C A_K\|_{L^2_\varphi(X)\to L^2_\varphi(X)} = \mathcal{O}(h^\infty). \tag{3-7}$$

In this sense the $A_F A_K$ remainder term is negligible. We again use (3-6) to write

$$\begin{aligned}(P-\lambda)G(\mathrm{Id} &- A_C - A_K - A_F + A_K A_C + A_C A_K + A_K A_F) \\ &= \mathrm{Id} - A_F A_K + A_C A_K A_C + A_F A_K A_C + A_K A_C A_K + A_C A_K A_F + A_K A_F A_K.\end{aligned}$$

Now all remainders but $A_C A_K A_C$, $A_K A_C A_K$, and $A_C A_K A_F$ are negligible in the sense of (3-7). Solving away again gives

$$\begin{aligned}(P-\lambda)G(\mathrm{Id} - A_C - A_K - A_F + A_K A_C + A_C A_K + A_K A_F - A_C A_K A_C - A_K A_C A_K - A_C A_K A_F) \\ = \mathrm{Id} - A_F A_K + A_F A_K A_C + A_K A_F A_K - A_K A_C A_K A_C \\ - A_C A_K A_C A_K - A_F A_K A_C A_K - A_K A_C A_K A_F.\end{aligned}$$

Now all remainders but $A_K A_C A_K A_C$ are negligible. Solving away one last time gives

$$
\begin{aligned}
(P-\lambda)G\big(\mathrm{Id} - A_C - A_K - A_F + A_K A_C + A_C A_K + A_K A_F \\
- A_C A_K A_C - A_K A_C A_K - A_C A_K A_F + A_K A_C A_K A_C\big) \\
= \mathrm{Id} - A_F A_K + A_C A_K A_C + A_F A_K A_C + A_K A_F A_K - A_C A_K A_C A_K \\
- A_F A_K A_C A_K - A_K A_C A_K A_F + A_C A_K A_C A_K A_C + A_F A_K A_C A_K A_C =: \mathrm{Id} + R,
\end{aligned}
$$

where R is defined by the equation, and $\|R\|_{L^2_\varphi(X)\to L^2_\varphi(X)} = \mathcal{O}(h^\infty)$. So for h small enough we may write, for $\operatorname{Im}\lambda > 0$,

$$
\begin{aligned}
(P-\lambda)^{-1} = G\big(\mathrm{Id} - A_C - A_K - A_F + A_K A_C + A_C A_K + A_K A_F \\
- A_C A_K A_C - A_K A_C A_K - A_C A_K A_F + A_K A_C A_K A_C\big)\sum_{k=0}^{\infty}(-R)^k.
\end{aligned}
$$

Combining this equation with (3-3), we see that $\chi(P-\lambda)^{-1}\chi$ continues to holomorphically to $|\operatorname{Re}\lambda| \le E$, $\operatorname{Im}\lambda \ge -\Gamma h$ and obeys

$$
\|\chi(P-\lambda)^{-1}\chi\|_{L^2_\varphi(X)\to H^2_{\varphi,h}(X)} \le C h^{-1-C_0|\operatorname{Im}\lambda|/h}. \qquad \square
$$

In summary, to prove (2-8) (and hence (1-1)), it remains to prove (3-3), (3-4) and (3-5).

3B. ***Statements of estimates for model operators.*** In this subsection we state six propositions: a resolvent estimate and a propagation of singularities estimate, for each of R_K, R_C, and R_F. Propositions 3.2, 3.4, and 3.6 imply (3-3) for $j = K$, C, and F, respectively. As we discuss after the statements, Propositions 3.3, 3.5, and 3.7 imply (3-4) and (3-5). The first two propositions concern R_K, and we prove them in Section 4. The next two concern R_C, and we prove them in Section 5. The last two concern R_F, and we prove them in Section 6. Hence at the end of Section 6 the proof of the Theorem will be complete.

Proposition 3.2. *For any $E \in (0,1)$ there is $C_0 > 0$ such that for any $M > 0$ there are $C, h_0 > 0$ such that*

$$
\|R_K(\lambda)\|_{L^2_\varphi(X)\to H^2_{\varphi,h}(X)} \le C \begin{cases} h^{-1} + |\lambda|, & \operatorname{Im}\lambda > 0, \\ h^{-1} e^{C_0|\operatorname{Im}\lambda|/h}, & \operatorname{Im}\lambda \le 0, \end{cases} \tag{3-8}
$$

for $|\operatorname{Re}\lambda| \le E$, $\operatorname{Im}\lambda \ge -Mh\log(1/h)$, $h \in (0, h_0]$.

Proposition 3.3. *Let $\Gamma \in \mathbb{R}$, $E \in (0,1)$. Let $A, B \in \Psi^0(X)$ have full symbols a and b with the projections to X of* $\operatorname{supp} a$ *and* $\operatorname{supp} b$ *compact and suppose that*

$$
\operatorname{supp} a \cap \left[\operatorname{supp} b \cup \bigcup_{t\ge 0} \exp(tH_p)\big[p^{-1}([-E,E]) \cap \operatorname{supp} b\big]\right] = \varnothing, \tag{3-9}
$$

where $\exp(tH_p)$ *is the bicharacteristic flow of p. Then, for any $N \in \mathbb{N}$,*

$$
\|A R_K(\lambda) B\|_{L^2_\varphi(X)\to H^2_{\varphi,h}(X)} = \mathcal{O}(h^\infty) \tag{3-10}
$$

for $|\operatorname{Re}\lambda| \le E$, $-\Gamma h \le \operatorname{Im}\lambda \le h^{-N}$.

Proposition 3.4. *For every $\chi \in C_0^\infty(X)$, $E \in (0,1)$, there is $C_0 > 0$ such that, for any $M > 0$, there are $h_0, C > 0$ such that the cutoff resolvent $\chi R_C(\lambda)\chi$ continues holomorphically from $\{\operatorname{Im}\lambda > 0\}$ to $\{|\operatorname{Re}\lambda| \le E, \operatorname{Im}\lambda \ge -Mh\}$, $h \in (0, h_0]$, and obeys*

$$\|\chi R_C(\lambda)\chi\|_{L^2_\varphi(X)\to H^2_{\varphi,h}(X)} \le C \begin{cases} h^{-1} + |\lambda|, & \operatorname{Im}\lambda > 0, \\ h^{-1-C_0|\operatorname{Im}\lambda|/h}, & \operatorname{Im}\lambda \le 0. \end{cases} \tag{3-11}$$

Proposition 3.5. *Let $r_0 < 0$, $\chi_- \in C_0^\infty((-\infty, r_0))$, $\chi_+ \in C_0^\infty((r_0, \infty))$, $\varphi \in C^\infty(\mathbb{R})$ supported in $(-\infty, 0)$ and bounded with all derivatives, $E \in (0,1)$, $\Gamma > 0$ be given. Then there exists $h_0 > 0$ such that*

$$\|\varphi(hD_r)\chi_+(r)R_C(\lambda)\chi_-(r)\|_{L^2_\varphi(X)\to H^2_{\varphi,h}(X)} = \mathcal{O}(h^\infty) \tag{3-12}$$

for $|\operatorname{Re}\lambda| \le E$, $-\Gamma h \le \operatorname{Im}\lambda \le h^{-N}$, $h \in (0, h_0]$.

Proposition 3.6. *For every $\chi \in C_0^\infty(X)$, $E \in (0,1)$, there is $C_0 > 0$ such that, for any $M > 0$, there are $h_0, C > 0$ such that the cutoff resolvent $\chi R_F(\lambda)\chi$ continues holomorphically from $\{\operatorname{Im}\lambda > 0\}$ to $\{|\operatorname{Re}\lambda| \le E, \operatorname{Im}\lambda \ge -Mh\log(1/h)\}$, $h \in (0, h_0]$, where it satisfies*

$$\|\chi R_F(\lambda)\chi\|_{L^2_\varphi(X)\to H^2_{\varphi,h}(X)} \le C \begin{cases} h^{-1} + |\lambda|, & \operatorname{Im}\lambda > 0, \\ h^{-1}e^{C_0|\operatorname{Im}\lambda|/h}, & \operatorname{Im}\lambda \le 0. \end{cases} \tag{3-13}$$

Proposition 3.7. *Let $r_0 > R_g$, $\chi_- \in C_0^\infty((-\infty, r_0))$, $\chi_+ \in C_0^\infty((r_0, \infty))$, $\varphi \in C^\infty(\mathbb{R})$ supported in $(0, \infty)$ and bounded with all derivatives, $E \in (0,1)$, $\Gamma > 0$ be given. Then there exists $h_0 > 0$ such that*

$$\|\chi_+(r)R_F(\lambda)\chi_-(r)\varphi(hD_r)\|_{L^2_\varphi(X)\to H^2_{\varphi,h}(X)} = \mathcal{O}(h^\infty) \tag{3-14}$$

for $|\operatorname{Re}\lambda| \le E$, $-\Gamma h \le \operatorname{Im}\lambda \le h^{-N}$, $h \in (0, h_0]$.

We conclude the subsection by deducing (3-4) and (3-5) from the above propositions.

Take $\varphi \in C^\infty(\mathbb{R})$, bounded with all derivatives and supported in $(0, \infty)$, and take $\tilde\chi_2, \tilde\chi_3 \in C_0^\infty(X)$ such that $\operatorname{supp}\tilde\chi_2 \subset \{r > R_g + 2\}$ and $\tilde\chi_3 \subset \{r < R_g + 2\}$, and such that $\tilde\chi_2\chi_2 = \chi_2\tilde\chi_2 = \chi_2$ and $\tilde\chi_3\chi_3 = \chi_3\tilde\chi_3 = \chi_3$. Then (3-4) follows from

$$\|\tilde\chi_3 R_F \tilde\chi_2 \varphi(hD_r)\|_{L^2_\varphi(X)\to H^2_{\varphi,h}(X)} + \|\tilde\chi_2(\operatorname{Id} - \varphi(hD_r))R_K\chi_1\|_{L^2_\varphi(X)\to H^2_{\varphi,h}(X)} = \mathcal{O}(h^\infty). \tag{3-15}$$

The estimate on the first term follows from (3-14), while the estimate on the second term follows from (3-10) if $\operatorname{supp}(1-\varphi)$ is contained in a sufficiently small neighborhood of $(-\infty, 0]$; it suffices to take a neighborhood small enough that no bicharacteristic in $p^{-1}([-E, E])$ goes from $T^*\operatorname{supp}\chi_1$ to $(T^*\operatorname{supp}\tilde\chi_2)\cap\operatorname{supp}(1-\varphi(\rho))$, where ρ is the dual variable to r in T^*X, and such a neighborhood exists by (2-4) because when a bicharacteristic leaves $T^*\operatorname{supp}\chi_1$ it has $\rho \ge 0$, and (2-4) gives a minimum amount by which ρ must grow in the time it takes the bicharacteristic to reach $T^*\operatorname{supp}\tilde\chi_2$. An analogous argument reduces (3-5) to (3-12): the analog of (3-15) is

$$\|\tilde\chi_3 R_K(\operatorname{Id} - \varphi(hD_r))\tilde\chi_2\|_{L^2_\varphi(X)\to H^2_{\varphi,h}(X)} + \|\varphi(hD_r)\tilde\chi_2 R_C\chi_1\|_{L^2_\varphi(X)\to H^2_{\varphi,h}(X)} = \mathcal{O}(h^\infty),$$

where $\varphi \in C^\infty(\mathbb{R})$ is bounded with all derivatives and supported in $(-\infty, 0)$, and $\tilde{\chi}_2,\ \tilde{\chi}_3 \in C_0^\infty(X)$ have $\operatorname{supp} \tilde{\chi}_2 \subset \{r > -R_g - 2\}$ and $\tilde{\chi}_3 \subset \{r < -R_g - 2\}$, and such that $\tilde{\chi}_2 \chi_2 = \chi_2 \tilde{\chi}_2 = \chi_2$ and $\tilde{\chi}_3 \chi_3 = \chi_3 \tilde{\chi}_3 = \chi_3$.

4. Model operator in the nonsymmetric region

In this section we prove Propositions 3.2 and 3.3. Although the techniques involved are all essentially well known, we go over them in some detail here because they are important in the more complicated analysis of P_C and P_F below.

4A. ***Proof of Proposition 3.2.*** This is similar to the argument in [Sjöstrand and Zworski 2007, §4]. Fix

$$E_0 \in (E, 1), \quad \varepsilon = 10 M h \log(1/h).$$

We will use the assumption that the flow is nontrapping to construct an *escape function* $q \in C_0^\infty(T^*X)$, that is to say a function such that

$$H_p q \le -1 \quad \text{near } T^* \operatorname{supp}(1 - W_K) \cap p^{-1}([-E_0, E_0]). \tag{4-1}$$

The construction will be given below. Then let $Q \in \Psi^{-\infty}(X)$ be a quantization of q, and

$$P_{K,\varepsilon} = e^{\varepsilon Q/h} P_K e^{-\varepsilon Q/h} = P_K - \varepsilon [P_K, Q/h] + \varepsilon^2 R,$$

where $R \in \Psi^{-\infty}(X)$ (see (2-26)). We will prove that

$$\|(P_{K,\varepsilon} - E')^{-1}\|_{L^2_\varphi(X) \to H^2_{\varphi,h}(X)} \le 5/\varepsilon, \quad E' \in [-E_0, E_0], \tag{4-2}$$

from which it follows, using first the openness of the resolvent set and then (2-23), that

$$\|(P_K - \lambda)^{-1}\|_{L^2_\varphi(X) \to H^2_{\varphi,h}(X)} \le \frac{h^{-N}}{M \log(1/h)}, \quad |\operatorname{Re} \lambda| \le E_0,\ |\operatorname{Im} \lambda| \le M h \log(1/h), \tag{4-3}$$

where

$$N = 10 M (\|Q\|_{H^2_{\varphi,h}(X) \to H^2_{\varphi,h}(X)} + \|Q\|_{L^2_\varphi(X) \to L^2_\varphi(X)}) + 1.$$

Then we will show how to use complex interpolation to improve (4-3) to (3-8).

Construction of $q \in C_0^\infty(T^*X)$ satisfying (4-1). As in [Vasy and Zworski 2000, §4], we take q of the form

$$q = \sum_{j=1}^{J} q_j, \tag{4-4}$$

where each q_j is supported near a bicharacteristic in $T^* \operatorname{supp}(1 - W_K) \cap p^{-1}([-E_0, E_0])$.

First, for each $\wp \in T^* \operatorname{supp}(1 - W_K) \cap p^{-1}([-E_0, E_0])$, define the following *escape time*:

$$T_\wp = \inf\{T \in \mathbb{R} : |t| \ge T - 1 \implies \exp(t H_p)\wp \notin T^* \operatorname{supp}(1 - W_K)\}.$$

Then put

$$T = \max\{T_\wp : \wp \in T^* \operatorname{supp}(1 - W_K) \cap p^{-1}([-E_0, E_0])\}.$$

Note that the nontrapping assumption in Section 2A implies that $T < \infty$. Let $\mathcal{S}_\wp$ be a hypersurface through $\wp$, transversal to H_p near $\wp$. If $U_\wp$ is a small enough neighborhood of $\wp$, then

$$V_\wp = \{\exp(tH_p)\wp' : \wp' \in U_\wp \cap \mathcal{S}_\wp, |t| < T + 1\}$$

is diffeomorphic to $\mathbb{R}^{2n-1} \times (-T-1, T+1)$ with $\wp$ mapped to $(0,0)$. Denote this diffeomorphism by $(y_\wp, t_\wp)$. Further shrinking $U_\wp$ if necessary, we may assume the inverse image of $\mathbb{R}^{2n-1} \times \{|t| \geq T\}$ is disjoint from $T^* \operatorname{supp}(1 - W_K)$. Then take $\varphi \in C_0^\infty(\mathbb{R}^{2n-1}; [0,1])$ identically 1 near 0, and $\chi \in C_0^\infty((-T-1, T+1))$ with $\chi' = -1$ near $[-T, T]$, and put

$$q_\wp = \varphi(y_\wp)\chi(t_\wp), \quad H_p q_\wp = \varphi(y_\wp)\chi'(t_\wp).$$

Note $H_p q_\wp \leq 0$ on $T^* \operatorname{supp}(1 - W_K)$ because $\chi' = -1$ there. Let $V'_\wp$ be the interior of $\{H_p q_\wp = -1\}$, note that the $V'_\wp$ cover $T^*(1 - W_K) \cap p^{-1}([-E_0, E_0])$, and extract a finite subcover $\{V'_{\wp_1}, \dots, V'_{\wp_J}\}$. Then put $q_j = q_{\wp_j}$ and define q by (4-4), so that

$$H_p q = \sum_{j=1}^{J} \varphi(y_{\wp_j})\chi'_\wp(t_{\wp_j}).$$

Then $H_p q \leq -1$ near $T^*(1 - W_K) \cap p^{-1}([-E_0, E_0])$ because at each point at least one summand is, and the other summands are nonpositive. □

Proof of (4-2). Let $\chi_0 \in C_0^\infty(X; [0,1])$ be identically 1 on a large enough set that $\chi_0 Q = Q\chi_0 = Q$. In particular we have $(1 - \chi_0)W_K = 1 - \chi_0$, allowing us to write

$$\|(1-\chi_0)u\|^2_{L^2_\varphi(X)} = -\operatorname{Im}\langle (P_{K,\varepsilon} - E')(1-\chi_0)u, (1-\chi_0)u\rangle_{L^2_\varphi(X)}.$$

Hence

$$\|(1-\chi_0)u\|_{L^2_\varphi(X)} \leq \|(P_{K,\varepsilon} - E')u\|_{L^2_\varphi(X)} + \|[P_{K,\varepsilon}, \chi_0]u\|_{L^2_\varphi(X)}.$$

To estimate $\|\chi_0 u\|_{L^2_\varphi(X)}$ and the remainder term $\|[P_{K,\varepsilon}, \chi_0]u\|_{L^2_\varphi(X)}$ we introduce a microlocal cutoff $\phi \in C_0^\infty(T^*X)$ which is identically 1 near $T^* \operatorname{supp}(1 - W_K) \cap p^{-1}([-E_0, E_0])$ and is supported in the interior of the set where $H_p q \leq -1$. Since the principal symbol of $P_{K,\varepsilon} - E'$ is

$$p_{K,\varepsilon} - E' = p - iW_K - E' - i\varepsilon\{p - iW_K, q\},$$

we have

$$|p_{K,\varepsilon} - E'| \geq 1 - E_0 \quad \text{near} \quad \operatorname{supp}(1 - \phi)$$

for $|E'| \leq E_0$, provided h (and hence ε) is sufficiently small. Then if $\Phi \in \Psi^{-\infty}(X)$ is a quantization of ϕ, we find using the semiclassical elliptic estimate (2-21) that

$$\|(\operatorname{Id} - \Phi)\chi_0 u\|_{H^2_{\varphi,h}(X)} \leq C\big(\|(P_{K,\varepsilon} - E')u\|_{L^2_\varphi(X)} + h\|u\|_{H^1_{\varphi,h}(X)}\big).$$

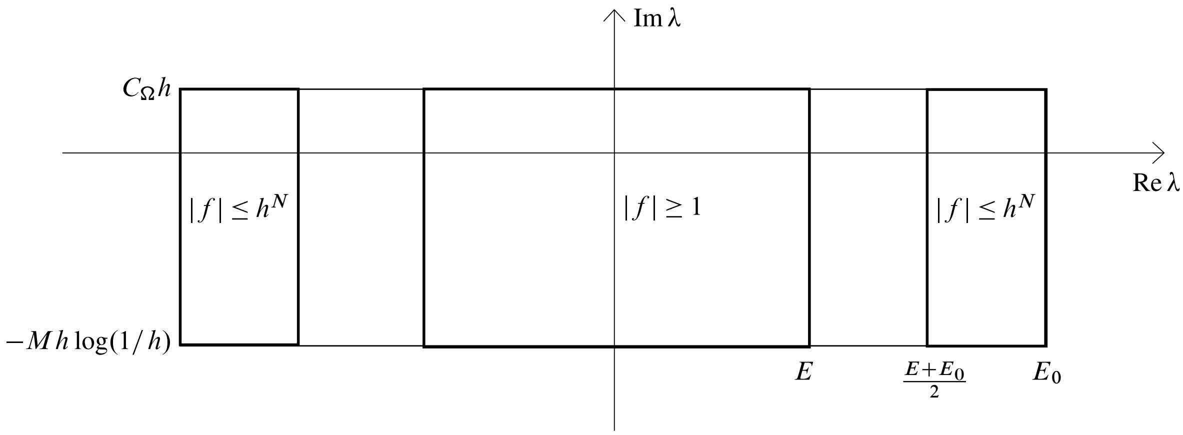

Figure 4. Bounds on f used in the complex interpolation argument.

Since $H_p q \leq -1$ near $\operatorname{supp}\phi$ we see that

$$\operatorname{Im} p_{K,\varepsilon} - E' = -W_K - \varepsilon\{p, q\} \leq -\varepsilon \quad \text{near} \quad \operatorname{supp}\phi.$$

Then, using the sharp Gårding inequality (2-22), we find that

$$\begin{aligned}\|(P_{K,\varepsilon} - E')\Phi\chi_0 u\|_{L^2_\varphi(X)} \|\Phi\chi_0 u\|_{L^2_\varphi(X)} &\geq -\langle \operatorname{Im}(P_{K,\varepsilon} - E')\Phi\chi_0 u, \Phi\chi_0 u\rangle_{L^2_\varphi(X)} \\ &\geq \varepsilon\|\Phi\chi_0 u\|^2_{L^2_\varphi(X)} - Ch\|u\|^2_{H^{1/2}_{\varphi,h}(X)}.\end{aligned}$$

This implies that

$$\begin{aligned}\|u\|_{L^2_\varphi(X)} &\leq \|(1-\chi_0)u\|_{L^2_\varphi(X)} + \|\Phi\chi_0 u\|_{L^2_\varphi(X)} + \|(\operatorname{Id} - \Phi)\chi_0 u\|_{L^2_\varphi(X)} \\ &\leq C\|(P_{K,\varepsilon} - E')u\|_{L^2_\varphi(X)} + \varepsilon^{-1}\|(P_{K,\varepsilon} - E')u\|_{L^2_\varphi(X)} + Ch^{1/2}\|u\|_{H^1_{\varphi,h}(X)}.\end{aligned}$$

As in the proof of (3-2), combining this with

$$\begin{aligned}\|u\|_{H^2_{\varphi,h}(X)} &\leq 3\|u\|_{L^2_\varphi(X)} + \|(P - E')u\|_{L^2_\varphi(X)} \\ &\leq 4\|u\|_{L^2_\varphi(X)} + \|(P_{K,\varepsilon} - E')u\|_{L^2_\varphi(X)} + C\varepsilon\|u\|_{L^2_\varphi(X)},\end{aligned} \tag{4-5}$$

we obtain (4-2) for h sufficiently small. ☐

Proof that (4-3) *implies* (3-8). We follow the approach of [Tang and Zworski 1998] as presented in [Nakamura, Stefanov and Zworski 2003, Lemma 3.1]. Observe first that (3-2) implies (3-8) for $\operatorname{Im}\lambda \geq C_\Omega h$ for any $C_\Omega > 0$.

Let $f(\lambda, h)$ be holomorphic in λ for $\lambda \in \Omega = [-E_0, E_0] + i[-Mh\log(1/h), C_\Omega h]$ and bounded uniformly in h there. Suppose further that, for $\lambda \in \Omega$,

$$|\operatorname{Re}\lambda| \leq E \implies |f| \geq 1, \quad |\operatorname{Re}\lambda| \in \left[\tfrac{1}{2}(E + E_0), E_0\right] \implies |f| \leq h^N.$$

For example, we may take f to be a characteristic function convolved with a gaussian:

$$f(\lambda,h)=\frac{2}{\sqrt{\pi}}\log(1/h)\int_{-\widetilde{E}}^{\widetilde{E}}\exp\bigl(-\log^2(1/h)(\lambda-y)^2\bigr)\,dy$$
$$=\operatorname{erfc}\bigl(\log(1/h)(\lambda-\widetilde{E})\bigr)-\operatorname{erfc}\bigl(\log(1/h)(\lambda+\widetilde{E})\bigr),$$

where $\widetilde{E}=\frac{1}{4}(3E+E_0)$, $\operatorname{erfc} z=2\int_z^\infty e^{-t^2}\,dt/\sqrt{\pi}$. We bound $|f|$ using the identity $\operatorname{erfc}(z)+\operatorname{erfc}(-z)=2$ and the fact that $\operatorname{erfc} z=\pi^{-1/2}z^{-1}e^{-z^2}(1+\mathcal{O}(z^{-2}))$ for $|\arg z|<\frac{3\pi}{4}$.

Then the subharmonic function

$$g(\lambda,h)=\log\|(P_K-\lambda)^{-1}\|_{L^2_\varphi(X)\to H^2_{\varphi,h}(X)}+\log|f(\lambda,h)|+\frac{N\operatorname{Im}\lambda}{Mh}$$

obeys

$$g\le C\quad\text{on }\partial\Omega\cap(\{|\operatorname{Re}\lambda|=E_0\}\cup\{\operatorname{Im}\lambda=-Mh\log(1/h)\})$$

and

$$g\le C+\log(1/h)\quad\text{on }\partial\Omega\cap\{\operatorname{Im}\lambda=C_\Omega h\}.$$

From the maximum principle and the lower bound on $|f|$ we obtain

$$\log\|(P_K-\lambda)^{-1}\|_{L^2_\varphi(X)\to H^2_{\varphi,h}(X)}+\frac{N\operatorname{Im}\lambda}{Mh}\le C+\log(1/h),$$

for $\lambda\in\Omega$, $|\operatorname{Re}\lambda|\le E$, from which (3-8) follows for $\lambda\in\Omega$. □

4B. ***Proof of Proposition 3.3.*** This is similar to [Datchev and Vasy 2012a, Lemma 5.1]. By (2-21), without loss of generality we may assume that a is supported in a neighborhood of $p^{-1}([-E,E])\cap\operatorname{supp}(1-W_K)$ which is as small as we please (but independent of h). In particular we may assume $\operatorname{supp} a$ is compact.

We will show that if $(P_K-\lambda)u=Bf$ with $\|f\|_{L^2_\varphi(X)}=1$, and if $\|A_0u\|\le Ch^k$ for some $A_0\in\Psi^0(X)$ with full symbol a_0 such that

$$a_0=1\quad\text{near }\operatorname{supp} a\cap p^{-1}([-E,E]),\qquad \operatorname{supp} a_0\cap\bigcup_{t\ge 0}\exp(tH_p)\operatorname{supp} b=\varnothing,$$

then $\|A_1u\|\le Ch^{k+1/2}$ for each $A_1\in\Psi^0(X)$ with full symbol a_1 satisfying $a_0=1$ near $\operatorname{supp} a_1$. Then the conclusion (3-10) follows by induction; the base step is given by (3-8).

Let $q\in C_0^\infty(T^*X;[0,\infty))$ such that

$$a_0=1\quad\text{near }\operatorname{supp} q,\qquad H_p(q^2)\le-(2\Gamma+1)q^2\quad\text{near }\operatorname{supp} a_1,\tag{4-6}$$
$$H_pq\le 0\quad\text{on }T^*\operatorname{supp}(1-W_K).\tag{4-7}$$

The construction of q is very similar to that of the function q used in the proof of Proposition 3.2 above, and is also given in [loc. cit.]. Write

$$H_p(q^2)=-\ell^2+r,$$

where $\ell, r \in C_0^\infty(T^*X)$ satisfy

$$\ell^2 \geq (2\Gamma+1)q^2, \quad \operatorname{supp} r \subset \{W_K = 1\}. \tag{4-8}$$

Let $Q, L, R \in \Psi^{-\infty}(X)$ have principal symbols q, ℓ, r respectively. Then

$$i[P, Q^*Q] = -hL^*L + hR + h^2F + R_\infty,$$

where $F \in \Psi^{-\infty}(X)$ has full symbol supported in $\operatorname{supp} q$ and $R_\infty \in h^\infty\Psi^{-\infty}(X)$. From this we conclude that

$$\begin{aligned}\|Lu\|^2_{L^2_\varphi(X)} &= -\frac{2}{h}\operatorname{Im}\langle Q^*QPu, u\rangle_{L^2_\varphi(X)} + \langle Ru, u\rangle_{L^2_\varphi(X)} + h\langle Fu, u\rangle_{L^2_\varphi(X)} + \mathcal{O}(h^\infty)\|u\|^2_{L^2_\varphi(X)} \\ &= -\frac{2}{h}\operatorname{Im}\langle Q^*Q(P_K-\lambda)u, u\rangle_{L^2_\varphi(X)} - \operatorname{Re}\langle Q^*QW_Ku, u\rangle_{L^2_\varphi(X)} - \frac{2}{h}\operatorname{Im}\lambda\|Qu\|^2_{L^2_\varphi(X)} \\ &\qquad + \langle Ru, u\rangle_{L^2_\varphi(X)} + h\langle Fu, u\rangle_{L^2_\varphi(X)} + \mathcal{O}(h^\infty)\|u\|^2_{L^2_\varphi(X)}.\end{aligned} \tag{4-9}$$

We now estimate the right-hand side of (4-9) term by term to prove that

$$\|Lu\|^2_{L^2_\varphi(X)} \leq 2\Gamma\|Qu\|^2_{L^2_\varphi(X)} + Ch\|A_0u\|^2_{L^2_\varphi(X)} + \mathcal{O}(h^\infty)\|u\|^2_{L^2_\varphi(X)}. \tag{4-10}$$

Indeed, since $\operatorname{supp} q \cap \operatorname{supp} b = \varnothing$ and since $(P_K-\lambda)u = Bf$ it follows that

$$\langle Q^*Q(P_K-\lambda)u, u\rangle_{L^2_\varphi(X)} = \mathcal{O}(h^\infty)\|u\|^2_{L^2_\varphi(X)}.$$

Next, we write

$$-\operatorname{Re}\langle Q^*QW_Ku, u\rangle_{L^2_\varphi(X)} = -\operatorname{Re}\langle W_KQu, Qu\rangle_{L^2_\varphi(X)} + \langle Q^*[W_K, Q]u, u\rangle_{L^2_\varphi(X)},$$

and observe that the first term is nonpositive because $W_K \geq 0$, and the second term is bounded by $Ch\|A_0u\|^2_{L^2_\varphi(X)}$. Since $\operatorname{Im}\lambda \geq -\Gamma h$ we have

$$-\frac{2}{h}\operatorname{Im}\lambda\|Qu\|^2_{L^2_\varphi(X)} \leq 2\Gamma\|Qu\|^2_{L^2_\varphi(X)},$$

while since $W_K = 1$ on $\operatorname{supp} r$ we have the elliptic estimate

$$\langle Ru, u\rangle_{L^2_\varphi(X)} = C\|R(P_K-\lambda)u\|_{L^2_\varphi(X)}\|u\|_{L^2_\varphi(X)} + Ch\|A_0u\|^2_{L^2_\varphi(X)},$$

and the first term is $\mathcal{O}(h^\infty)\|u\|^2_{L^2_\varphi(X)}$ since $\operatorname{supp} r \cap \operatorname{supp} b = \varnothing$. Finally $h\langle Fu, u\rangle_{L^2_\varphi(X)} \leq Ch\|A_0u\|^2$ by the inductive hypothesis, giving (4-10).

But by (4-8) and the sharp Gårding inequality we have

$$\langle (D^*D - (2\Gamma+1)Q^*Q)u, u\rangle \geq -Ch\|A_0u\|^2 - \mathcal{O}(h^\infty)\|u\|^2.$$

Hence by the inductive hypothesis we have

$$\|Qu\|^2 \leq Ch^{2k+1}\|u\|^2,$$

completing the inductive step.

5. Model operator in the cusp

In this section we prove Propositions 3.4 and 3.5. We begin by separating variables over the eigenspaces of Δ_{S_-}, writing

$$P_C = \bigoplus_{m=0}^{\infty} h^2 D_r^2 + (h\lambda_m)^2 e^{-2(r+\beta(r))} + h^2 V(r) - 1 - i W_C(r),$$

where $0 = \lambda_0 < \lambda_1 \le \cdots$ are square roots of the eigenvalues of Δ_{S_-}. Roughly speaking, it suffices to prove (3-11), (3-12) with P_C replaced by $P(\alpha)$, with estimates uniform in $\alpha \in \{0\} \cup [h\lambda_1, \infty)$, where

$$P(\alpha) = h^2 D_r^2 + \alpha^2 e^{-2(r+\beta(r))} + h^2 V(r) - 1 - i W_C(r).$$

The precise estimates for these operators which imply Propositions 3.4 and 3.5 are stated in Lemmas 5.1, 5.2, and 5.3 below.

5A. ***The case $\alpha = 0$.*** The analysis of $(P(0) - \lambda)^{-1}$ is very similar to that of R_K in Section 4. The only additional technical ingredient is the method of complex scaling, which for this operator works just as in [Sjöstrand and Zworski 1991; 2007].

Lemma 5.1. *For every $\chi \in C_0^\infty(X)$, $E \in (0,1)$, there is $C_0 > 0$ such that, for any $M > 0$, there exist $h_0, C > 0$ such that the cutoff resolvent $\chi(P(0)-\lambda)^{-1}\chi$ continues holomorphically from $\{\operatorname{Im}\lambda > 0\}$ to $\{|\operatorname{Re}\lambda| \le E, \operatorname{Im}\lambda \ge -Mh\log(1/h)\}$, $h \in (0, h_0]$, and obeys*

$$\|\chi(P(0)-\lambda)^{-1}\chi\|_{L^2(\mathbb{R})\to H_h^2(\mathbb{R})} \le Ch^{-1} e^{C_0|\operatorname{Im}\lambda|/h}. \tag{5-1}$$

Let $r_0 \in \mathbb{R}$, $\chi_- \in C_0^\infty((-\infty, r_0))$, $\chi_+ \in C_0^\infty((r_0,\infty))$, $\varphi \in C^\infty(\mathbb{R})$ supported in $(-\infty, 0)$ and bounded with all derivatives, $\Gamma > 0$ be given. Then there exists $h_0 > 0$ such that

$$\|\varphi(hD_r)\chi_+(r)(P(0)-\lambda)^{-1}\chi_-(r)\|_{L^2(\mathbb{R})\to H_h^2(\mathbb{R})} = \mathcal{O}(h^\infty) \tag{5-2}$$

for $|\operatorname{Re}\lambda| \le E$, $-\Gamma h \le \operatorname{Im}\lambda \le h^{-N}$, $h \in (0, h_0]$.

Proof of (5-1). We use complex scaling to replace $P(0)$ by the complex scaled operator $P_\delta(0)$, defined below. As we will see, $P_\delta(0)$ is semiclassically elliptic for $|r|$ sufficiently large and obeys (5-1) without cutoffs.

We have

$$P(0) = h^2 D_r^2 + h^2 V(r) - 1 - i W_C(r).$$

Fix $R > R_g$ sufficiently large that

$$\operatorname{supp}\chi \cup \operatorname{supp}\chi_+ \cup \operatorname{supp}\chi_- \subset (-R, \infty). \tag{5-3}$$

Let $\gamma \in C^\infty(\mathbb{R})$ be nondecreasing and obey $\gamma(r) = 0$ for $r \ge -R$, $\gamma'(r) = \tan\theta_0$ for $r \le -R-1$ (here θ_0 is as in Section 2A), and impose further that $\beta(r)$ is holomorphic near $r + i\delta\gamma(r)$ for every $r < -R$, $\delta \in (0,1)$. Below we will take $\delta \ll 1$ independent of h.

Now put

$$P_\delta(0) = \frac{h^2 D_r^2}{(1+i\delta\gamma'(r))^2} - h\frac{\delta\gamma''(r) h D_r}{(1+i\delta\gamma'(r))^3} + h^2 V(r+i\delta\gamma(r)) - 1 - i W_C(r+i\delta\gamma(r)).$$

If we define the differential operator with complex coefficients

$$\widetilde{P}(0) = h^2 D_z^2 + h^2 V(z) - 1 - i W_C(z),$$

where z varies in $\{z = r + i\delta\gamma(r) : \ r \in \mathbb{R}, \ \delta \in (0,1)\}$, and where $W_C(z) := 0$ whenever $\operatorname{Im} z \neq 0$, then we have

$$P(0) = \widetilde{P}(0)|_{\{z=r:r\in\mathbb{R}\}}, \quad P_\delta(0) = \widetilde{P}(0)|_{\{z=r+i\delta\gamma(r):r\in\mathbb{R}\}}. \tag{5-4}$$

We will show that if $\chi_0 \in C^\infty(\mathbb{R})$ has $\operatorname{supp}\chi_0 \cap \operatorname{supp}\gamma = \varnothing$, then

$$\chi_0(P(0)-\lambda)^{-1}\chi_0 = \chi_0(P_\delta(0)-\lambda)^{-1}\chi_0, \quad \operatorname{Im}\lambda > 0. \tag{5-5}$$

From this it follows that if one of these operators has a holomorphic continuation to any domain, then so does the other, and the continuations agree, so that it suffices to prove (5-1) and (5-2) with $P(0)$ replaced by $P_\delta(0)$. To prove (5-5) we will prove that if

$$(P(0)-\lambda)u = v \quad \text{and} \quad (P_\delta(0)-\lambda)u_\delta = v$$

for $v \in L^2(\mathbb{R})$ with $\operatorname{supp} v \subset \{r : \gamma(r) = 0\}$, and $u, u_\delta \in L^2(\mathbb{R})$, then

$$u|_{\{r:\gamma(r)=0\}} = u_\delta|_{\{r:\gamma(r)=0\}}.$$

Thanks to (5-4), it suffices to show that if $\tilde{u}$ solves $(\widetilde{P}(0)-\lambda)\tilde{u} = v$ with $\tilde{u}|_{\{z=r:r\in\mathbb{R}\}} \in L^2(\mathbb{R})$, then $\tilde{u}|_{\{z=r+i\delta\gamma(r):r\in\mathbb{R}\}} \in L^2(\mathbb{R})$. For the proof of this statement we may take λ fixed with $\operatorname{Re}\lambda = 0$ since the general statement follows by holomorphic continuation.

Observe that for $\operatorname{Re} z < -R$, we have

$$(\widetilde{P}(0)-\lambda)\tilde{u}(z) = 0. \tag{5-6}$$

We will use the WKB method to construct solutions $u_\pm$ to (5-6) which are exponentially growing or decaying as $\operatorname{Re} z \to -\infty$. Define

$$f(z) = V(z) - (1+\lambda)/h^2, \quad \varphi(z) = (4f(z)f''(z) - 5f'(z)^2)(16f(z))^{-5/2}.$$

Now (see, e.g., [Olver 1974, Chapter 6, Theorem 11.1]) there exist two solutions to (5-6) given by

$$u_\pm(z) = f(z)^{-1/4} e^{\pm\int_{\gamma_{z,-R}}\sqrt{f(z')}dz'}(1+b_\pm(z)), \quad \operatorname{Re} z < -R,$$

taking principal branches of the roots and with the contour of integration $\gamma_{z,-R}$ taken from z to $-R$ such that $\sqrt{\operatorname{Re} z'}$ is monotonic along $\gamma_{z,-R}$. The functions $b_\pm$ obey

$$|b_\pm(z)| \le \exp(\max(|\varphi(z')| : z' \in \gamma_\pm)) - 1 \le Ch$$

when $\operatorname{Re} z > R$, where γ_+ and γ_- are contours from $-\infty$ to z and from z to $-R$, respectively, such that $\sqrt{\operatorname{Re} z'}$ is monotonic along the contour. It follows that, for fixed h sufficiently small,

$$|u_+(z)| \le Ce^{\operatorname{Re} z/C}, \quad |u_-(z)| \ge Ce^{-\operatorname{Re} z/C}$$

for $\operatorname{Re} z < -R$. Hence $\tilde{u}|_{\{z=r:r\in\mathbb{R}\}} \in L^2(\mathbb{R})$ implies that $\tilde{u}$ is proportional to u_+. This implies that $\tilde{u}|_{\{z=r+i\delta\gamma(r):r\in\mathbb{R}\}} \in L^2(\mathbb{R})$, completing the proof of (5-5).

Fix

$$E_0 \in (E, 1), \quad \varepsilon = 10Mh\log(1/h).$$

The semiclassical principal symbol of $P_\delta(0)$ is

$$p_\delta(0) = \frac{\rho^2}{(1+i\delta\gamma'(r))^2} - 1 = \rho^2(1+\mathcal{O}(\delta)) - 1. \tag{5-7}$$

In this case the escape function can be made more explicit: we take $q \in C_0^\infty(T^*\mathbb{R})$ with

$$q(r,\rho) = -4r\rho(1-E_0)^{-2}, \quad H_{p_\delta(0)}q = -8\rho^2(1-E_0)^{-2}(1+\mathcal{O}(\delta)) \tag{5-8}$$

on $\{|r| \le R+1,\ |\rho| \le 2\}$. Let $Q \in \Psi^{-\infty}(\mathbb{R})$ be a quantization of q and put

$$P_{\delta,\varepsilon}(0) = e^{\varepsilon Q/h} P_\delta(0) e^{-\varepsilon Q/h} = P_\delta(0) - \varepsilon[P_\delta(0), Q/h] + \varepsilon^2 R,$$

where $R \in \Psi^{-\infty}(\mathbb{R})$ (see (2-26)). We will prove

$$\|(P_{\delta,\varepsilon}(0) - E')^{-1}\|_{L^2(\mathbb{R})\to H_h^2(\mathbb{R})} \le 5/\varepsilon, \quad E' \in [-E_0, E_0], \tag{5-9}$$

from which it follows by (2-23) that

$$\|(P_\delta(0)-\lambda)^{-1}\|_{L^2(\mathbb{R})\to H_h^2(\mathbb{R})} \le \frac{h^{-N}}{M\log(1/h)}, \quad |\operatorname{Re}\lambda| \le E_0,\ |\operatorname{Im}\lambda| \le Mh\log(1/h), \tag{5-10}$$

where $N = 10M(\|Q\|_{H_h^2(\mathbb{R})\to H_h^2(\mathbb{R})} + \|Q\|_{L^2(\mathbb{R})\to L^2(\mathbb{R})}) + 1$. As before we will use complex interpolation to improve (5-10) to

$$\|(P_\delta(0)-\lambda)^{-1}\|_{L^2(\mathbb{R})\to H_h^2(\mathbb{R})} \le Ch^{-1}e^{C|\operatorname{Im}\lambda|/h} \tag{5-11}$$

for $-E \le \operatorname{Re}\lambda \le E$, $\operatorname{Im}\lambda > -Mh\log(1/h)$. Combining (5-5) and (5-11) gives (5-1).

Let $\phi \in C_0^\infty(\mathbb{R};[0,1])$ have $\phi(\rho) = 1$ for $|\rho|$ near $[1-E_0, 1+E_0]$ and $\operatorname{supp}\phi \subset \left\{\tfrac{1}{2}(1-E_0) < |\rho| < 2\right\}$. By (5-7), if δ is small enough and h is small enough depending on δ, then on $\operatorname{supp}(1-\phi(\rho))$ we have $|p_{\delta,\varepsilon}(0) - E'| \ge \delta(1+\rho^2)/C$, uniformly in $E' \in [-E_0, E_0]$ and in h, where $p_{\delta,\varepsilon}(0)$ is the semiclassical principal symbol of $P_{\delta,\varepsilon}(0)$. Hence, by the semiclassical elliptic estimate (2-18),

$$\|(\operatorname{Id}-\phi(hD_r))u\|_{H_h^2(\mathbb{R})} \le C\delta^{-1}\|(P_{\delta,\varepsilon}(0)-E')(\operatorname{Id}-\phi(hD_r))u\|_{L^2(\mathbb{R})} + \mathcal{O}(h^\infty)\|u\|_{H_h^{-N}(\mathbb{R})}.$$

On $\operatorname{supp}\phi(\rho)$ we use the negativity of the imaginary part of the principal symbol of $P_{\delta,\varepsilon}(0)$. Indeed, on $\{(r,\rho) : \rho \in \operatorname{supp}\phi,\ |r| \le R+1\}$ we have, using (5-8),

$$\operatorname{Im} p_{\delta,\varepsilon}(0) = \operatorname{Im} p_\delta(0) + \operatorname{Im} i\varepsilon H_{p_{\delta,\varepsilon}(0)}q = \frac{-2\delta\gamma'(r)\rho^2}{|1+i\delta\gamma'(r)|^4} - \frac{8\varepsilon\rho^2}{(1-E_0)^2}(1+\mathcal{O}(\delta)) \le -\varepsilon,$$

provided δ is sufficiently small. Meanwhile, on $\{(r,\rho):\rho\in\operatorname{supp}\phi,\ |r|\ge R+1\}$ we have

$$\operatorname{Im} p_{\delta,\varepsilon}(0)=\operatorname{Im} p_\delta(0)+\operatorname{Im} i\varepsilon H_{p_{\delta,\varepsilon}(0)}q=\frac{-2\delta\tan\theta_0\rho^2}{|1+i\delta\tan\theta_0|^4}+\mathcal{O}(\varepsilon)\le-\delta/C,$$

provided h (and hence ε) is sufficiently small.

Then, using the sharp Gårding inequality (2-19), we have, for h sufficiently small,

$$\begin{aligned}\|\varphi(hD_r)u\|_{L^2(\mathbb{R})}\|(P_{\delta,\varepsilon}(0)-E')\varphi(hD_r)u\|_{L^2(\mathbb{R})}&\ge-\langle\operatorname{Im}(P_{\delta,\varepsilon}(0)-E')\varphi(hD_r)u,\varphi(hD_r)u\rangle_{L^2(\mathbb{R})}\\&\ge\varepsilon\|\varphi(hD_r)u\|^2_{L^2(\mathbb{R})}-Ch\|u\|^2_{H_h^{1/2}(\mathbb{R})}.\end{aligned}$$

We deduce (5-9) from this just as we did (4-2) above.

To improve (5-10) to (5-11) we use almost the same complex interpolation argument as we did to improve (4-3) to (3-8). The only difference is that in the first step we note that

$$\operatorname{Im} p_\delta(0)=\frac{-2\delta\gamma'(r)}{|1+i\delta\gamma'(r)|^4}\le 0,$$

so by the sharp Gårding inequality (2-19) we have, for some $C_\Omega>0$,

$$\langle\operatorname{Im} P_\delta(0)u,u\rangle_{L^2(\mathbb{R})}\ge-C_\Omega h\|u\|^2_{L^2(\mathbb{R})},$$

so that $\|(P_\delta(0)-\lambda)^{-1}\|_{L^2(\mathbb{R})}\le 1/C_\Omega h$, when $\operatorname{Im}\lambda\ge 2C_\Omega h$. □

Proof of (5-2). Let $(P_\delta(0)-\lambda)u=f$, where $\|f\|_{L^2(\mathbb{R})}=1$, $\operatorname{supp} f\subset\operatorname{supp}\chi_-$ and $P_\delta(0)$ is as in the proof of (5-1). We must show that

$$\|\varphi(hD_r)\chi_+(r)u\|_{H_h^2(\mathbb{R})}=\mathcal{O}(h^\infty);\tag{5-12}$$

recall that the replacement of $P(0)$ by $P_\delta(0)$ is justified by (5-5). To prove (5-12) we use an argument by induction based on a nested sequence of escape functions.

More specifically, take

$$q=\varphi_r(r)\varphi_\rho(\rho),\quad H_{p_\delta(0)}q=2\rho\varphi_r'(r)\varphi_\rho(\rho)+\mathcal{O}(\delta),$$

where $\varphi_r\in C_0^\infty(\mathbb{R};[0,\infty))$ with $\operatorname{supp}\varphi_r\subset(r_0,\infty)$, $\varphi_r'\ge 0$ near $[r_0,R+1]$ (here R is as in (5-3)), $\varphi_r'>0$ near $\operatorname{supp}\chi_+$. Take $\varphi_\rho\in C_0^\infty(\mathbb{R};[0,\infty))$ with $\operatorname{supp}\varphi_\rho\subset(-\infty,0)$, $\varphi_\rho'\le 0$ near $[-2,0]$, $\varphi_\rho\ne 0$ near $\operatorname{supp}\varphi\cap[-2,0]$. Impose further that $\sqrt{\varphi}_r,\sqrt{\varphi}_\rho\in C_0^\infty(\mathbb{R})$, and that $\varphi_r'\ge c\varphi_r$ for $r\le R+1$, where $c>0$ is chosen large enough that $H_{p_0(\delta)}q\le-(2\Gamma+1)q$ on $\{r\le R+1,\rho\ge-2\}$; see Figure 5.

We will show that if $\|A_0u\|_{L^2(\mathbb{R})}\le Ch^k$ for $A_0\in\Psi^0(\mathbb{R})$ with full symbol supported sufficiently near $\operatorname{supp} q$ and for some $k\in\mathbb{R}$, then $\|A_1u\|_{L^2(\mathbb{R})}\le Ch^{k+1/2}$ for $A_1\in\Psi^0(\mathbb{R})$ with full symbol supported sufficiently near $\{r\in\operatorname{supp}\chi_+,\rho\in\operatorname{supp}\varphi\}$. The conclusion (5-12) then follows by induction. (The base step of the induction follows from (5-11) or even from (5-10).)

In the remainder of the proof all norms and inner products are in $L^2(\mathbb{R})$ and we omit the subscript for brevity.

We write

$$H_{p_\delta(0)}q^2=-b^2+e,$$

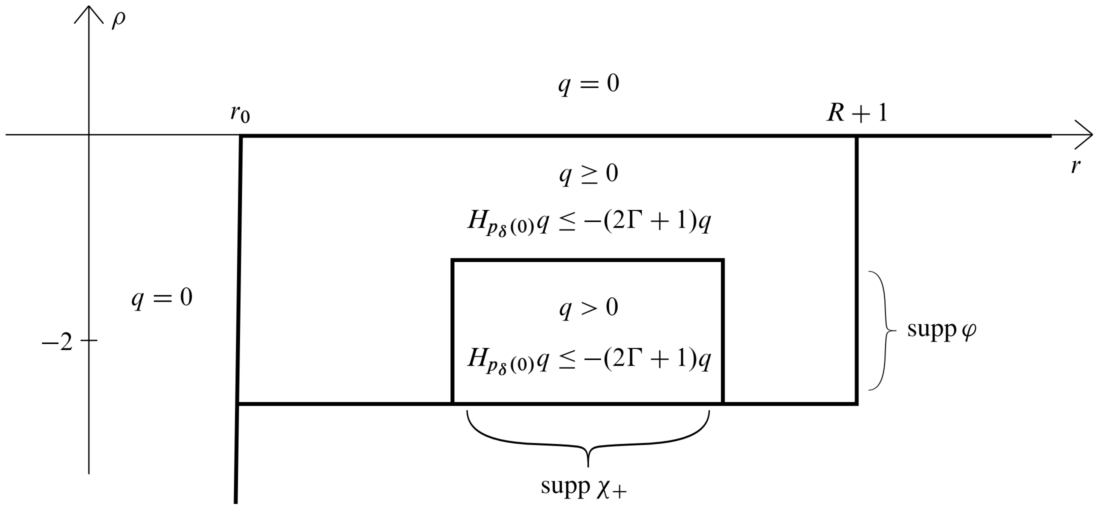

Figure 5. The escape function q used to prove propagation of singularities (5-2) in the case $\alpha = 0$. The derivative along the flow lines $H_{p_\delta(0)}q$ is negative and provides ellipticity for our positive commutator argument near $\{r \in \operatorname{supp}\chi_+, \rho \in \operatorname{supp}\varphi\}$. We allow $H_{p_\delta(0)}q > 0$ (the unfavorable sign for us) only in $\{r > R+1\}$ and in $\{\rho < -2\}$, because in this region $p_\delta(0)$ is elliptic.

where $b, e \in C_0^\infty(T^*\mathbb{R})$, $b > 0$ near $\{r \in \operatorname{supp}\chi_+, \rho \in \operatorname{supp}\varphi, -2 \leq \rho\}$, $b^2 \geq (2\Gamma+1)q^2$ everywhere, and $\operatorname{supp} e \cap (\{r \leq R+1, \rho \geq -2\} \cup \{r \leq r_0\}) = \varnothing$. Let Q, B, E be quantizations of q, b, e respectively. Then

$$i[P_\delta(0), Q^*Q] = -hB^*B + hE + h^2F,$$

where $F \in \Psi^0(\mathbb{R})$ has full symbol supported in $\operatorname{supp} q$. From this we conclude that

$$\|Bu\|^2 = -\frac{2}{h}\operatorname{Im}\langle Q^*Q(P_\delta(0)-\lambda)u, u\rangle - \frac{2}{h}\operatorname{Im}\lambda\|Qu\|^2 + \langle Eu, u\rangle + h\langle Fu, u\rangle + \mathcal{O}(h^\infty)\|u\|^2.$$

From $(P_\delta(0)-\lambda)u = f$ and $\operatorname{WF}_h' Q \cap T^* \operatorname{supp} f = \varnothing$ it follows that the first term is $\mathcal{O}(h^\infty)\|u\|^2$. Similarly $\operatorname{WF}_h' E \cap (\operatorname{supp} f \cup p_\delta^{-1}(0)) = \varnothing$ implies by (2-18) that the third term is $\mathcal{O}(h^\infty)\|u\|^2$. The fourth term is bounded by $Ch^{2k+1}\|u\|^2$ by the inductive hypothesis, giving

$$\|Bu\|^2 \leq 2\Gamma\|Qu\|^2 + Ch^{2k+1}\|u\|^2.$$

By (2-19) we have

$$\langle (B^*B - (2\Gamma+1)Q^*Q)u, u\rangle \geq -Ch\|Ru\|^2,$$

where $R \in \Psi_0^{0,0}(\mathbb{R})$ is microsupported in an arbitrarily small neighborhood of $\operatorname{WF}_h' Q$. Hence $\|Ru\| \leq Ch^k\|u\|$ and we have

$$\|Qu\|^2 \leq Ch^{2k+1}\|u\|^2,$$

completing the inductive step and also the proof. □

5B. ***The case $\alpha \geq \lambda_1 h$.*** Propositions 3.4 and 3.5 follow from (5-1), (5-2) and the following two lemmas.

Lemma 5.2. *For any $E \in (0,1)$ there is $C_0 > 0$ such that for any $M, \lambda_1 > 0$ there are $h_0, C > 0$ such that if $h \in (0, h_0]$, $\alpha \geq \lambda_1 h$, $\lambda \in [-E, E] + i[-Mh, \infty)$, then*

$$\|(P(\alpha)-\lambda)^{-1}\|_{L^2(\mathbb{R})\to H_h^2(\mathbb{R})} \leq C \log(1/h) h^{-1-C_0|\operatorname{Im}\lambda|/h}. \tag{5-13}$$

If $\chi \in C^\infty(\mathbb{R})$ has $\chi' \in C_0^\infty(\mathbb{R})$ and $\chi(r) = 0$ for r sufficiently negative, then

$$\|\chi(P(\alpha)-\lambda)^{-1}\chi\|_{L^2(\mathbb{R})\to H_h^2(\mathbb{R})} \leq C h^{-1-2C_0|\operatorname{Im}\lambda|/h} \tag{5-14}$$

in the same range of h, α, λ, and with the same C_0 and h_0 (but with different C).

Lemma 5.3. *Let $r_0 < 0$, $\chi_- \in C_0^\infty((-\infty, r_0))$, $\chi_+ \in C_0^\infty((r_0, \infty))$, $\varphi \in C_0^\infty((-\infty, 0))$, $E \in (0,1)$, $\Gamma, \lambda_1, N > 0$ be given. Then there exists $h_0 > 0$ such that*

$$\|\varphi(hD_r)\chi_+(r)(P(\alpha)-\lambda)^{-1}\chi_-(r)\|_{L^2(\mathbb{R})\to H_h^2(\mathbb{R})} = \mathcal{O}(h^\infty) \tag{5-15}$$

uniformly for $\alpha \geq \lambda_1 h$, $\operatorname{Re}\lambda \in [-E, E]$, $-\Gamma h \leq \operatorname{Im}\lambda \leq h^{-N}$, $h \in (0, h_0]$.

Take $\alpha_0 > 0$ such that if $\alpha \geq \alpha_0$ and $r \leq 0$ then $\alpha^2 e^{-2(r+\beta(r))} \geq 3$. We consider the cases $\lambda_1 h \leq \alpha \leq \alpha_0$ and $\alpha_0 \leq \alpha$ separately.

Proof of (5-13), (5-14), *and* (5-15) *for $\alpha_0 \leq \alpha$.* In this case $P(\alpha)$ is "elliptic" (although not pseudodifferential in the usual sense because of the exponentially growing term $\alpha^2 e^{-2(r+\beta(r))}$) and better estimates hold. Use the fact that $W_C \geq 0$ and $\alpha^2 e^{-2(r+\beta(r))} \geq 3$ for $r \leq 0$ to write

$$\int_{-\infty}^0 |u|^2\,dr \leq \frac{1}{3}\int_{-\infty}^\infty \alpha^2 e^{-2(r+\beta(r))}|u|^2\,dr \leq \tfrac{1}{3}\operatorname{Re}\langle P(\alpha)u, u\rangle_{L^2(\mathbb{R})} + \left(\tfrac{1}{3} + \mathcal{O}(h^2)\right)\|u\|^2_{L^2(\mathbb{R})},$$
$$\int_0^\infty |u|^2\,dr = \int_0^\infty W_C|u|^2 dr \leq \int_{-\infty}^\infty W_C|u|^2\,dr = -\operatorname{Im}\langle P(\alpha)u, u\rangle_{L^2(\mathbb{R})}.$$

Adding the inequalities gives

$$\|u\|^2_{L^2(\mathbb{R})} \leq 2\|(P(\alpha)-\lambda)u\|_{L^2(\mathbb{R})}\|u\|_{L^2(\mathbb{R})} + \left(\tfrac{1}{3}\operatorname{Re}\lambda - \operatorname{Im}\lambda + \tfrac{1}{3} + \mathcal{O}(h^2)\right)\|u\|^2_{L^2(\mathbb{R})}.$$

So long as $\operatorname{Im}\lambda - \frac{1}{3}\operatorname{Re}\lambda + \frac{2}{3} \geq \epsilon$ for some $\epsilon > 0$, it follows that

$$\|u\|_{L^2(\mathbb{R})} \leq C\|(P(\alpha)-\lambda)u\|_{L^2(\mathbb{R})}. \tag{5-16}$$

To obtain (5-13) we observe that

$$\|h^2 D_r^2 u\|^2_{L^2(\mathbb{R})}$$
$$= \|(h^2 D_r^2 + \alpha^2 e^{-2(r+\beta(r))})u\|^2_{L^2(\mathbb{R})} - \|\alpha^2 e^{-2(r+\beta(r))}u\|^2_{L^2(\mathbb{R})} - 2\operatorname{Re}\langle h^2 D_r^2 u, \alpha^2 e^{-2(r+\beta(r))}u\rangle_{L^2(\mathbb{R})},$$

while

$$-\operatorname{Re}\langle h^2 D_r^2 u, \alpha^2 e^{-2(r+\beta(r))}u\rangle_{L^2(\mathbb{R})}$$
$$= -\|\alpha e^{-(r+\beta(r))}hD_r u\|^2_{L^2(\mathbb{R})} + 2\operatorname{Im}\langle hD_r u, (1+\beta'(r))h\alpha^2 e^{-2(r+\beta(r))}u\rangle_{L^2(\mathbb{R})},$$

so that

$$\|h^2 D_r^2 u\|_{L^2(\mathbb{R})} \le 2\|(h^2 D_r^2 + \alpha^2 e^{-2(r+\beta(r))})u\|_{L^2(\mathbb{R})} \le 2\|(P(\alpha)-\lambda)u\|_{L^2(\mathbb{R})} + C|\lambda|\|u\|_{L^2(\mathbb{R})}.$$

Together with (5-16), this implies (5-13) (and hence (5-14)) with the right-hand side replaced by $C(1+|\lambda|)$. The estimate (5-15) follows from the stronger Agmon estimate

$$\|\chi_+(r)(P(\alpha)-\lambda)^{-1}\chi_-(r)\|_{L^2(\mathbb{R})\to H_h^2(\mathbb{R})} = \mathcal{O}(e^{-1/(Ch)});$$

see for example [Zworski 2012, Theorems 7.3 and 7.1]. □

Proof of (5-13) *for* $\lambda_1 h \le \alpha \le \alpha_0$. For this range of α we use the following rescaling (I'm very grateful to Nicolas Burq for suggesting this rescaling):

$$\tilde r = r/\log(2\alpha_0/\alpha), \quad \tilde h = h/\log(2\alpha_0/\alpha). \tag{5-17}$$

In these variables we have

$$P(\alpha) = (\tilde h D_{\tilde r})^2 + 4\alpha_0^2 e^{-2[(1+\tilde r)\log(2\alpha_0/\alpha)+\tilde\beta(\tilde r)]} + \tilde h^2 \widetilde V(\tilde r) - 1 - i\widetilde W_C(\tilde r),$$

where

$$\tilde\beta(\tilde r) = \beta(r), \quad \widetilde V(\tilde r) = \log(2\alpha_0/\alpha)^2 V(r), \quad \widetilde W_C(\tilde r) = W_C(r).$$

We will show that

$$\|(P(\alpha)-\lambda)^{-1}\|_{L^2_{\tilde r}\to H^2_{h,\tilde r}} \le C\tilde h^{-1} e^{C_0|\operatorname{Im}\lambda|/\tilde h} \tag{5-18}$$

for $|\operatorname{Re}\lambda| \le E,\ \operatorname{Im}\lambda \ge -M\tilde h\log(1/\tilde h)$, from which (5-13) follows.

We now use a variant of the gluing argument in Section 3A to replace the exponentially growing term $4\alpha_0^2 e^{-2[(1+\tilde r)\log(\alpha_0/\alpha)+\tilde\beta(\tilde r)]}$ with a bounded one. Fix $\widetilde R > 0$ such that

$$\tilde r \le -\widetilde R,\ \alpha \le \alpha_0 \quad\Longrightarrow\quad \alpha_0^2 e^{-2[(1+\tilde r)\log(2\alpha_0/\alpha)+\tilde\beta(\tilde r)]} > 1.$$

Take $\widetilde V_B, \widetilde V_E \in C^\infty(\mathbb{R},[0,\infty))$ such that

$$\widetilde V_E(\tilde r) = 4\alpha_0^2 e^{-2[(1+\tilde r)\log(2\alpha_0/\alpha)+\tilde\beta(\tilde r)]} \quad \text{for } \tilde r \le -\widetilde R$$

and $\widetilde V_E(\tilde r) \ge 4$ for all $\tilde r$, while

$$\widetilde V_B(\tilde r) = 4\alpha_0^2 e^{-2[(1+\tilde r)\log(2\alpha_0/\alpha)+\tilde\beta(\tilde r)]} \quad \text{for } \tilde r \ge -\widetilde R - 3$$

and $\widetilde V_B$ is decreasing in $\tilde r$ and bounded together with all derivatives, uniformly in α (see Figure 6).

Let

$$P_E(\alpha) = (\tilde h D_{\tilde r})^2 + \widetilde V_E(\tilde r) + \tilde h^2\widetilde V(\tilde r) - 1 - i\widetilde W_C(\tilde r),$$
$$P_B(\alpha) = (\tilde h D_{\tilde r})^2 + \widetilde V_B(\tilde r) + \tilde h^2\widetilde V(\tilde r) - 1 - i\widetilde W_C(\tilde r),$$

and let $R_E = (P_E(\alpha)-\lambda)^{-1}$, $R_B = (P_B(\alpha)-\lambda)^{-1}$. Note that

$$\|R_E\|_{L^2_{\tilde r}\to H^2_{h,\tilde r}} \le C$$

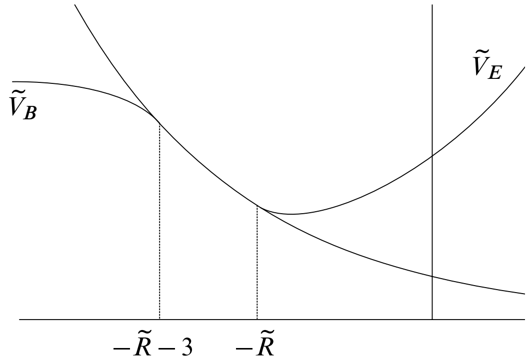

Figure 6. The model potentials $\widetilde{V}_E$ and $\widetilde{V}_B$. The former agrees with the function $4\alpha_0^2 e^{-2[(1+\tilde{r})\log(2\alpha_0/\alpha)+\tilde{\beta}(\tilde{r})]}$ for $\tilde{r} \le -\widetilde{R}$, and $\widetilde{V}_B$ agrees with the same function for $\tilde{r} \ge -\widetilde{R}-3$.

by the same proof as that of (5-13) for $\alpha \ge \alpha_0$. We will show that (5-18) follows from

$$\|R_B\|_{L^2_{\tilde{r}} \to H^2_{\tilde{h},\tilde{r}}} \le C\tilde{h}^{-1} e^{C_0|\operatorname{Im}\lambda|/\tilde{h}} \tag{5-19}$$

for $|\operatorname{Re}\lambda| \le E, \operatorname{Im}\lambda \ge -M\tilde{h}\log(1/\tilde{h})$. Indeed, let $\chi_E \in C^\infty(\mathbb{R};\mathbb{R})$ have $\chi_E(\tilde{r}) = 1$ near $\tilde{r} \le -\widetilde{R}-2$ and $\chi_E(\tilde{r}) = 0$ near $\tilde{r} \ge -\widetilde{R}-1$, and let $\chi_B = 1-\chi_E$. Let

$$G = \chi_E(\tilde{r}-1)R_E\chi_E(\tilde{r}) + \chi_B(\tilde{r}+1)R_B\chi_B(\tilde{r}).$$

Then

$$(P(\alpha)-\lambda)G = \operatorname{Id} + [\tilde{h}^2 D^2_{\tilde{r}}, \chi_E(\tilde{r}-1)]R_E\chi_E(\tilde{r}) + [\tilde{h}^2 D^2_{\tilde{r}}, \chi_B(\tilde{r}+1)]R_B\chi_B(\tilde{r}) = \operatorname{Id} + A_E + A_B.$$

As in Section 3A we have $A_E^2 = A_B^2 = 0$. We also have the Agmon estimate

$$\|A_E\|_{L^2_{\tilde{r}} \to L^2_{\tilde{r}}} \le e^{-1/(C\tilde{h})};$$

see for example [Zworski 2012, Theorems 7.3 and 7.1]. Solving away A_B using G we find that

$$(P(\alpha)-\lambda)G(\operatorname{Id} - A_B) = \operatorname{Id} + \mathcal{O}_{L^2_{\tilde{r}} \to L^2_{\tilde{r}}}(e^{-1/(C\tilde{h})}), \tag{5-20}$$

and since $\|G(\operatorname{Id} - A_B)\|_{L^2_{\tilde{r}} \to H^2_{\tilde{h},\tilde{r}}} \le C\tilde{h}^{-1} e^{C|\operatorname{Im}\lambda|/\tilde{h}}$, this implies (5-18).

The proof of (5-19) follows that of (5-1) with these differences: the $-i\widetilde{W}_C(\tilde{r})$ term removes the need for complex scaling, and the $\widetilde{V}_B(\tilde{r})$ term puts P_B in a mildly exotic operator class and leads to a slightly modified escape function q and microlocal cutoff ϕ. Fix

$$E_0 \in (E, 1), \quad \varepsilon = 10M\tilde{h}\log(1/\tilde{h}). \tag{5-21}$$

The $\tilde{h}$-semiclassical principal symbol of P_B (note that $P_B \in \Psi^2_\delta(\mathbb{R})$ for any $\delta > 0$) is

$$p_B = \tilde{\rho}^2 + \widetilde{V}_B(\tilde{r}) - 1 - i\widetilde{W}_C(\tilde{r}), \tag{5-22}$$

where $\tilde\rho$ is dual to $\tilde r$. Take $q \in C_0^\infty(T^*\mathbb{R})$ such that on $\{-\widetilde R \le \tilde r \le 0,\ |\tilde\rho| \le 2\}$ we have

$$q(\tilde r, \tilde\rho) = -C_q(\tilde r + \widetilde R + 1)\tilde\rho,$$
$$\operatorname{Re} H_{p_B} q = -2C_q\tilde\rho^2 + C_q(\tilde r + \widetilde R + 1)\widetilde V_B'(\tilde r) \le -C_q(\operatorname{Re} p_B + 1),$$

where $C_q > 0$ is a large constant which will be specified below, and where for the inequality we used (2-2). Let $Q \in \Psi^{-\infty}(\mathbb{R})$ be a quantization of q with $\tilde h$ as semiclassical parameter and put

$$P_{B,\varepsilon} = e^{\varepsilon Q/\tilde h} P_B e^{-\varepsilon Q/\tilde h} = P_B - \varepsilon[P_B, Q/\tilde h] + \varepsilon^2 \tilde h^{-4\delta} R, \tag{5-23}$$

where $R \in \Psi_\delta^{-\infty}(\mathbb{R})$ by (2-26). The $\tilde h$-semiclassical principal symbol of $P_{B,\varepsilon}$ is

$$p_{B,\varepsilon} = \tilde\rho^2 + V_B(\tilde r) - 1 - i\widetilde W_C(\tilde r) + i\varepsilon H_{p_B} q.$$

We will prove

$$\|(P_{B,\varepsilon} - E')^{-1}\|_{L^2_{\tilde r} \to H^2_{\tilde h,\tilde r}} \le 5/\varepsilon, \quad E' \in [-E_0, E_0], \tag{5-24}$$

from which it follows by (2-23) that

$$\|(P_{B,\varepsilon} - \lambda)^{-1}\|_{L^2_{\tilde r} \to H^2_{\tilde h,\tilde r}} \le \frac{\tilde h^{-N}}{M\log(1/\tilde h)}, \quad |\operatorname{Re}\lambda| \le E_0,\ |\operatorname{Im}\lambda| \le M\tilde h\log(1/\tilde h), \tag{5-25}$$

where

$$N = 10M(\|Q\|_{H^2_{\tilde h,\tilde r} \to H^2_{\tilde h,\tilde r}} + \|Q\|_{L^2_{\tilde r} \to L^2_{\tilde r}}) + 1.$$

The proof that (5-25) implies (5-19) is the same as the proof that (4-3) implies (3-8).

Let $\phi \in C_0^\infty(T^*\mathbb{R})$ be identically 1 near $\{(\tilde r, \tilde\rho) : -\widetilde R \le \tilde r \le 0,\ |\tilde\rho| \le 2,\ |\operatorname{Re} p_B(\tilde r, \tilde\rho)| \le E_0\}$ and be supported such that $\operatorname{Re} H_{p_B} q < 0$ on $\operatorname{supp}\phi$. Let Φ be the quantization of ϕ with $\tilde h$ as semiclassical parameter. For h (and hence $\tilde h$ and ε) small enough, we have $|p_{B,\varepsilon} - E'| \ge (1 + \tilde\rho^2)/C$ on $\operatorname{supp}(1-\phi)$, uniformly in $E' \in [-E_0, E_0]$, in $\alpha \le \alpha_0$ and in h. Hence, by the semiclassical elliptic estimate (2-18),

$$\|(\operatorname{Id} - \Phi)u\|_{H^2_{\tilde h,\tilde r}} \le C\|(P_{B,\varepsilon} - E')(\operatorname{Id} - \Phi)u\|_{L^2_{\tilde r}} + \mathcal{O}(h^\infty)\|u\|_{H^{-N}_{\tilde h,\tilde r}}.$$

Using the fact that $\operatorname{Re} H_{p_B} q < 0$ on $\operatorname{supp}\phi$, fix C_q large enough that on $\operatorname{supp}\phi$ we have

$$\operatorname{Im} p_{B,\varepsilon} = -\widetilde W_C(\tilde r) + \varepsilon \operatorname{Re} H_{p_B} q \le -\varepsilon.$$

Then, using the sharp Gårding inequality (2-19), we have, for h sufficiently small,

$$\begin{aligned}\|\Phi u\|_{L^2_{\tilde r}(\mathbb{R})}\|(P_{B,\varepsilon} - E')\Phi u\|_{L^2_{\tilde r}(\mathbb{R})} &\ge -\langle \operatorname{Im}(P_{B,\varepsilon} - E')\Phi u, \Phi u\rangle_{L^2_{\tilde r}(\mathbb{R})} \\ &\ge \varepsilon\|\Phi u\|^2_{L^2_{\tilde r}(\mathbb{R})} - C\tilde h^{1-2\delta}\|u\|^2_{H^{1/2}_{\tilde h,\tilde r}(\mathbb{R})}.\end{aligned}$$

We deduce (5-24) from this just as we did (4-2) above. □

Proof of (5-14) *for* $\lambda_1 h \le \alpha \le \alpha_0$.. It suffices to show that

$$\|\chi R_B \chi\|_{L^2_{\tilde r} \to H^2_{h,r}} \le C/h \tag{5-26}$$

when $|\mathrm{Re}\,\lambda| \le E_0$, $\mathrm{Im}\,\lambda \ge 0$, with R_B as in the proof of (5-13) for $\lambda_1 h \le \alpha \le \alpha_0$, E_0 as in (5-21).[1] Then $\|\chi(P(\alpha)-\lambda)^{-1}\chi\|_{L^2_r \to H^2_{h,r}} \le C/h$ (for the same range of parameters) follows by the same argument that reduced (5-13) to (5-19) above. After this, (5-14) follows by complex interpolation as in the proof that (4-3) implies (3-8) above. Indeed, take $f(\lambda, h)$ holomorphic in λ, bounded uniformly for $\lambda \in \Omega = [-E_0, E_0] + i[-Mh \log\log(1/h), 0]$, and satisfying

$$|\mathrm{Re}\,\lambda| \le E \implies |f| \ge 1, \quad |\mathrm{Re}\,\lambda| \le \left[\tfrac{1}{2}(E+E_0), E_0\right] \implies |f| \le h^2$$

for $\lambda \in \Omega$. Then define the subharmonic function

$$g(\lambda, h) = \log \|\chi(P(\alpha)-\lambda)^{-1}\chi\|_{L^2_r \to H^2_{h,r}} + \log|f(\lambda,h)| + 2C_0 \frac{\mathrm{Im}\,\lambda}{h} \log(1/h),$$

and apply the maximum principle to g on Ω, observing that $g \le C + \log(1/h)$ on $\partial\Omega$.

It now remains to prove (5-26), which we do using a "noncompact" variant of the positive commutator method of [Datchev and Vasy 2012b]. Fix $-R_0 < \inf \operatorname{supp} \chi$ and take $f \in L^2_r$ with $\operatorname{supp} f \subset (-R_0, \infty)$. Let $u = R_B f$. We will show that $\|\chi u\|_{H^2_{h,r}} \le C\|f\|_{L^2_r}/h$.

As an escape function take $q \in S^0(\mathbb{R})$ with $q \ge 0$ everywhere and such that

$$q(r,\rho) = \begin{cases} 1 + 2R_0 e^{-1/R_0}, & -R_0 \ge r, \\ 1 + 2R_0 e^{-1/R_0} - \rho(r + R_0 + 1)e^{-1/(r+R_0)}, & -R_0 < r \le 0 \text{ and } |\rho| \le 2. \end{cases}$$

We do not prescribe additional conditions on q outside of this range of (r,ρ), as P_B is semiclassically elliptic there. The h-semiclassical principal symbol of P_B is (see (5-22))

$$p_B = \rho^2 + V_B(r) - 1 - iW_C(r),$$

where $V_B(r) = \widetilde{V}_B(\tilde{r})$. Making $-\widetilde{R}$ more negative if necessary, we may suppose without loss of generality that

$$r \ge -R_0 \quad \implies \quad V_B(r) = \alpha^2 e^{-2(r+\beta(r))}.$$

For $r \le -R_0$ we have $H_{p_B} q = 0$, and for $-R_0 < r \le 0$, $|\rho| \le 2$ we have

$$\begin{aligned} \mathrm{Re}\, H_{p_B} q(r,\rho) &= \left[-2\rho^2(1 + 1/(r+R_0)) + V_B'(r)(r+R_0+1)\right] e^{-1/(r+R_0)} \\ &\le -(\mathrm{Re}\, p_B + 1)e^{-1/(r+R_0)}. \end{aligned}$$

Consequently, we may write

$$\mathrm{Re}\, H_{p_B}(q^2) = -b^2 + a,$$

where $a, b \in C_0^\infty(T^*\mathbb{R})$ and $\operatorname{supp} a$ is disjoint from $\{r \le -R_0\}$ and from $\{-R_0 < r \le 0\} \cap \{|\rho| \le 2\}$. Note that

$$b \ne 0 \quad \text{on } \{|p_B| \le E_0\} \cap T^*(-R_0, 0). \tag{5-27}$$

Let $Q = \mathrm{Op}(q)$ as in (2-15). Then

$$i[P_B, Q^*Q] = -hB^*B + hA + [W_C, Q^*Q] + h^2 Y, \tag{5-28}$$

[1] Note that for this proof we do not use the variables $\tilde{r}$ and $\tilde{h}$.

where $B, A, Y \in \Psi^{-\infty}(\mathbb{R})$ and B, A have semiclassical principal symbols b, a. Note that if $\chi_0 \in C_0^\infty((-R_0, \infty))$, then by (5-27) and (2-18) we have

$$\|\chi_0 u\|^2_{H^2_{h,r}} \le C(\|Bu\|^2_{L^2_r} + \log^2(1/h)\|f\|^2_{L^2_r}), \tag{5-29}$$

so it suffices to show that

$$\|Bu\|^2_{L^2_r} \le Ch^{-2}\|f\|^2_{L^2_r}. \tag{5-30}$$

Combining (5-28) with

$$\langle i[P_B, Q^*Q]u, u\rangle_{L^2_r} = -2\,\mathrm{Im}\langle Q^*Qu, f\rangle_{L^2_r} + 2\langle W_C Q^*Qu, u\rangle_{L^2_r} + 2\,\mathrm{Im}\,\lambda\|Qu\|^2_{L^2_r}$$

gives

$$\begin{aligned}\|Bu\|^2_{L^2_r} = \langle Au, u\rangle_{L^2_r} + \frac{2}{h}\mathrm{Im}\langle Q^*Qu, f\rangle_{L^2_r} - \frac{1}{h}\langle (W_C Q^*Q + Q^*QW_C)u, u\rangle_{L^2_r}\\ - \frac{2\,\mathrm{Im}\,\lambda}{h}\|Qu\|^2_{L^2_r} + h\langle Yu, u\rangle_{L^2_r}.\end{aligned} \tag{5-31}$$

We now estimate the right-hand side term by term to obtain (5-30). Since $P_B - \lambda$ is semiclassically elliptic on $\mathrm{supp}\, a$, by (2-18) followed by (5-13) we have

$$|\langle Au, u\rangle_{L^2_r}| \le C\|f\|^2_{L^2_r} + Ch^2\|u\|^2_{L^2_r} \le C\log^2(1/h)\|f\|^2_{L^2_r}.$$

For any $\epsilon > 0$ and $\chi_1 \in C_0^\infty(\mathbb{R})$ with $\chi_1 = 1$ near $\mathrm{supp}\, f$ we have

$$\frac{2}{h}\mathrm{Im}\langle Q^*Qu, f\rangle_{L^2_r} \le \epsilon\|\chi_1 u\|^2_{L^2_r} + \frac{C}{h^2\epsilon}\|f\|^2_{L^2_r}.$$

By (5-27) and the elliptic estimate (2-18), if further $\inf\mathrm{supp}\,\chi_1 > -R_0$, then (5-29) gives

$$\frac{2}{h}\mathrm{Im}\langle Q^*Qu, f\rangle_{L^2_r} \le C\epsilon\|Bu\|^2_{L^2_r} + \frac{C}{h^2\epsilon}\|f\|^2_{L^2_r}.$$

Next we have, using $W_C \ge 0$ and the fact that $h^{-1}[W_C, Q^*]Q$ has imaginary principal symbol, followed by (5-13),

$$\begin{aligned}-\frac{1}{h}\langle (W_C Q^*Q + Q^*QW_C)u, u\rangle_{L^2_r} &= -\frac{2}{h}\langle W_C Qu, Qu\rangle_{L^2_r} + \frac{2}{h}\mathrm{Re}\langle [W_C, Q^*]Qu, u\rangle_{L^2_r}\\ &\le Ch\|u\|^2_{L^2_r} \le C\frac{\log^2(1/h)}{h}\|f\|^2_{L^2_r}.\end{aligned}$$

Finally we observe that $-2\,\mathrm{Im}\,\lambda\|Qu\|^2_{L^2_r}/h \le 0$ since $\mathrm{Im}\,\lambda \ge 0$, while (5-13) implies

$$h\langle Yu, u\rangle_{L^2_r} \le C\frac{\log^2(1/h)}{h}\|f\|^2_{L^2_r}.$$

This completes the estimation of (5-31) term by term, giving (5-30). □

Proof of (5-15) *for* $\lambda_1 h \le \alpha \le \alpha_0$. We begin this proof with the same rescaling to $\tilde{r}$ and $\tilde{h}$, and the same parametrix construction as for the proof of (5-13) for $\lambda_1 h \le \alpha \le \alpha_0$ above, but with the additional requirement that

$$-\widetilde{R} \le r_0/\log 2.$$

Then if we put

$$\widetilde{\chi}_+(\tilde{r}) = \chi_+(r), \quad \widetilde{\chi}_-(\tilde{r}) = \chi_-(r),$$

we have

$$\operatorname{supp} \widetilde{\chi}_+ \subset (r_0/\log(2\alpha_0/\alpha), \infty) \subset (r_0/\log 2, \infty), \quad \operatorname{supp} \chi_E \subset (-\infty, -\widetilde{R}-1),$$

and hence

$$\widetilde{\chi}_+(\tilde{r})\chi_E(\tilde{r}-1) = 0. \tag{5-32}$$

Then, noting that (5-20) implies

$$(P(\alpha)-\lambda)^{-1} = G(\mathrm{Id} - A_B)(\mathrm{Id} + \mathcal{O}_{L^2_{\tilde{r}} \to L^2_{\tilde{r}}}(e^{-1/(C\tilde{h})})),$$

we use (5-32) to write

$$\widetilde{\chi}_+(\tilde{r})(P(\alpha)-\lambda)^{-1}\widetilde{\chi}_-(\tilde{r}) = \widetilde{\chi}_+(\tilde{r}) R_B \widetilde{\chi}_-(\tilde{r}) + \mathcal{O}_{L^2_{\tilde{r}} \to H^2_{\tilde{h},\tilde{r}}}(e^{-1/(C\tilde{h})}).$$

Returning to the r and h variables, we see that it suffices to show that

$$\|\varphi(hD_r)\chi_+(r) R_B \chi_-(r)\|_{L^2_r \to H^2_{h,r}} = \mathcal{O}(h^\infty). \tag{5-33}$$

The proof of (5-33) is almost the same as that of (5-2). There are two differences.

The first difference is that as an escape function we use

$$q = \varphi_r(r)\varphi_\rho(\rho), \quad \operatorname{Re} H_{p_B} q = 2\rho\varphi_r'(r)\varphi_\rho(\rho) - V_C'(r)\varphi_r'(r)\varphi_\rho'(\rho),$$

where $\varphi_r \in C_0^\infty(\mathbb{R};[0,\infty))$ with $\operatorname{supp}\varphi_r \subset (r_0,\infty)$, $\varphi_r' \ge 0$ near $[r_0, 0]$, $\varphi_r' > 0$ near $\operatorname{supp}\chi_+$. Take $\varphi_\rho \in C_0^\infty(\mathbb{R};[0,\infty))$ with $\operatorname{supp}\varphi_\rho \subset (-\infty, 0)$, $\varphi_\rho' \le 0$ near $[-2, 0]$, $\varphi_\rho \ne 0$ near $\operatorname{supp}\varphi \cap [-2, 0]$. Impose further that $\sqrt{\varphi_r}, \sqrt{\varphi_\rho} \in C_0^\infty(\mathbb{R})$, and that $\varphi_r' \ge c\varphi_r$ for $r \le 0$, where $c > 0$ is chosen large enough that $\operatorname{Re} H_{p_B} q \le -(2\Gamma+1)q$ on $\{r \le 0, \rho \ge -2\}$.

The second difference is that the complex absorbing barrier W_C produces a remainder term in the positive commutator estimate, analogous to the one in the proof of (5-14) for $\lambda_1 h \le \alpha \le \alpha_0$ above. The same argument removes the remainder term in this case. □

6. Model operator in the funnel

In this section we prove Propositions 3.6 and 3.7. As in Section 5, we begin by separating variables over the eigenspaces of Δ_{S_+}, writing

$$P_F = \bigoplus_{m=0}^{\infty} h^2 D_r^2 + (1 - W_F(r))(h\lambda_m)^2 e^{-2(r+\beta(r))} + h^2 V(r) - 1 - iW_F(r),$$

where $0 = \lambda_0 < \lambda_1 \le \cdots$ are square roots of the eigenvalues of Δ_{S_+}. Roughly speaking, it suffices to prove (3-13), (3-14) with P_F replaced by $P(\alpha)$, with estimates uniform in $\alpha \ge 0$, where

$$P(\alpha) = h^2 D_r^2 + (1 - W_F(r))\alpha^2 e^{-2(r+\beta(r))} + h^2 V(r) - 1 - i W_F(r).$$

More specifically, with notation as in those two propositions, (3-13) follows from

$$\|\chi(P(\alpha)-\lambda)^{-1}\chi\|_{L^2(\mathbb{R})\to H_h^2(\mathbb{R})} \le C \begin{cases} h^{-1} + |\lambda|, & \operatorname{Im}\lambda > 0, \\ h^{-1} e^{C_0|\operatorname{Im}\lambda|/h}, & \operatorname{Im}\lambda \le 0, \end{cases} \tag{6-1}$$

and (3-14) follows from

$$\|\chi_+(r)(P(\alpha)-\lambda)^{-1}\chi_-(r)\varphi(hD_r)\|_{L^2(\mathbb{R})\to H_h^2(\mathbb{R})} = \mathcal{O}(h^\infty), \tag{6-2}$$

so in this section we will prove (6-1) and (6-2).

To do that we use a variant of the method of complex scaling presented in the proof of Lemma 5.1, but with contours γ depending on α in such a way as to give estimates uniform in α; the α-dependence is needed because the term $\alpha^2(1 - W_F(r))e^{-2(r+\beta(r))}$, although exponentially decaying, is not uniformly exponentially decaying as $\alpha \to \infty$. Such contours were first used in [Zworski 1999, §4]; here we present a simplified approach based on that in [Datchev 2010, §5.2].

Fix $R > R_g$ sufficiently large that

$$\operatorname{supp}\chi \cup \operatorname{supp}\chi_+ \cup \operatorname{supp}\chi_- \subset (-\infty, R)$$

and that

$$\operatorname{Re} z \ge R,\ 0 \le \arg z \le \theta_0 \quad \Longrightarrow \quad |\operatorname{Im}\beta(z)| \le \tfrac{1}{2}|\operatorname{Im} z|, \tag{6-3}$$

where θ_0 is as in Section 2A. Let $\gamma = \gamma_\alpha(r)$ be real-valued, smooth in r with $\gamma'(r) \ge 0$ for all r, and obey $\gamma(r) = 0$ for $r \le R$ (here and below $\gamma' = \partial_r\gamma$). Suppose $\gamma'' \in C_0^\infty(\mathbb{R})$ for each α, but not necessarily uniformly in α. Now put

$$P_\gamma(\alpha) = \frac{h^2 D_r^2}{(1+i\gamma'(r))^2} - h\frac{\gamma''(r) h D_r}{(1+i\gamma'(r))^3} + \alpha^2(1 - W_F(r))e^{-2(r+i\gamma(r)+\beta(r+i\gamma(r)))} \\ + h^2 V(r + i\gamma(r)) - 1 - i W_F(r).$$

If we define the differential operator with complex coefficients

$$\widetilde{P}(\alpha) = h^2 D_z^2 + \alpha^2(1 - W_F(z))e^{-2(z+\beta(z))} + h^2 V(z) - 1 - i W_F(z),$$

where z varies in $\{z = r + i\delta\gamma(r) : r \in \mathbb{R},\ \delta \in (0,1)\}$, and where $W_F(z) := 0$ whenever $\operatorname{Im} z \ne 0$, then we have

$$P(\alpha) = \widetilde{P}(\alpha)|_{\{z=r:r\in\mathbb{R}\}}, \quad P_\gamma(\alpha) = \widetilde{P}(\alpha)|_{\{z=r+i\gamma(r):r\in\mathbb{R}\}}.$$

If $\chi_0 \in C^\infty(\mathbb{R})$ has $\operatorname{supp}\chi_0 \cap \operatorname{supp}\gamma = \varnothing$, then

$$\chi_0(P(\alpha)-\lambda)^{-1}\chi_0 = \chi_0(P_\gamma(\alpha)-\lambda)^{-1}\chi_0, \quad \operatorname{Im}\lambda > 0,$$

by an argument almost identical to that used to prove (5-5); the only difference is we construct WKB solutions which are exponentially growing and decaying as $\operatorname{Re} z \to +\infty$ rather than $-\infty$, and we take $f(z) = (\alpha^2 e^{-2(z+\beta(z))} + h^2 V(z) - 1 - \lambda)/h^2$.

Consequently, to prove (6-1) and (6-2), it is enough to show that

$$\|(P_\gamma(\alpha) - \lambda)^{-1}\|_{L^2(\mathbb{R}) \to H_h^2(\mathbb{R})} \le C e^{C_0 |\operatorname{Im} \lambda|/h} \tag{6-4}$$

and

$$\|\chi_+(r)(P_\gamma(\alpha) - \lambda)^{-1} \chi_-(r) \varphi(h D_r)\|_{L^2(\mathbb{R}) \to H_h^2(\mathbb{R})} = \mathcal{O}(h^\infty) \tag{6-5}$$

for a suitably chosen γ, with estimates uniform in $\alpha \ge 0$.

Fix $R_- > R$ such that

$$|\operatorname{Im} \beta(z)| \le \tfrac{1}{2} \operatorname{Im} z \tag{6-6}$$

for $\operatorname{Re} z \ge R_-$, $0 \le \arg z \le \theta_0$, with θ_0 as in Section 2A. Take $\alpha_0 > 0$ such that

$$\alpha_0^2 e^{-2(R+1)} e^{-2 \max |\operatorname{Re} \beta|} = 8, \tag{6-7}$$

where $\max |\operatorname{Re} \beta|$ is taken over $\mathbb{R} \cup \{|z| > R_g,\ 0 \le \arg z \le \theta_0\}$. We consider the cases $\alpha \le \alpha_0$ and $\alpha \ge \alpha_0$ separately.

Proof of (6-4) *for* $0 \le \alpha \le \alpha_0$. Fix

$$E_0 \in (E, 1), \quad \varepsilon = 10 M h \log(1/h).$$

We use the same complex scaling as in the proof of Lemma 5.1. In this range γ is independent of α and we put $\gamma = \delta \gamma_-$, where $0 < \delta \ll 1$ will be specified later, and we require $\gamma_-(r) = 0$ for $r \le R_-$, $\gamma_-'(r) \ge 0$ for all r, and $\gamma_-'(r) = \tan \theta_0$ for $r \ge R_- + 1$.

The semiclassical principal symbol of $P_\gamma(\alpha)$ is

$$\begin{aligned} p_\gamma(\alpha) &= \frac{\rho^2}{(1 + i\gamma'(r))^2} + \alpha^2 (1 - W_F(r)) e^{-2(r + i\gamma(r) + \beta(r + i\gamma(r)))} - 1 - i W_F(r) \\ &= \rho^2 + \alpha^2 (1 - W_F(r)) e^{-2(r + \beta(r))} - 1 - i W_F(r) + \mathcal{O}(\delta), \end{aligned}$$

where the implicit constant in $\mathcal{O}$ is uniform in compact subsets of $T^*\mathbb{R}$. Moreover,

$$\operatorname{Re} p_\gamma(\alpha) + 1 \ge \rho^2 - \mathcal{O}(\delta),$$

and, using (6-6),

$$\begin{aligned} \operatorname{Im} p_\gamma(\alpha) &\le -\alpha^2 (1 - W_F(r)) e^{-2(r + \operatorname{Re} \beta(r + i\gamma(r))} \sin(2(\gamma(r) + \operatorname{Im} \beta(r + i\gamma(r)))) \\ &\le -\alpha^2 (1 - W_F(r)) e^{-2(r + \operatorname{Re} \beta(r + i\gamma(r))} \sin \gamma(r) \\ &= -\alpha^2 (1 - W_F(r)) e^{-2(r + \operatorname{Re} \beta(r + i\gamma(r))} \gamma(r) (1 + \mathcal{O}(\delta^2)), \end{aligned} \tag{6-8}$$

again uniformly on compact subsets of $T^*\mathbb{R}$. Take $q \in C_0^\infty(T^*\mathbb{R})$ such that on $\{0 \le r \le R_- + 1,\ |\rho| \le 2\}$ we have

$$\begin{aligned} q &= -C_q(r+1)\rho, \\ \frac{\operatorname{Re} H_{p_\gamma} q}{C_q} &= -2\rho^2 - (W_F'(r) + 2(1+\beta'(r))(r+1)\alpha^2 e^{-2(r+\beta(r))} + \mathcal{O}(\delta) \\ &\le -(\operatorname{Re} p_\gamma + 1) \le -\rho^2 + \mathcal{O}(\delta), \end{aligned}$$

where $C_q > 0$ will be specified later, and provided δ is sufficiently small. Let $Q = \operatorname{Op}(q)$ and put

$$P_{\gamma,\varepsilon}(\alpha) = e^{\varepsilon Q/h} P_\gamma(\alpha) e^{-\varepsilon Q/h} = P_\gamma(\alpha) - \varepsilon[P_\gamma(\alpha), Q/h] + \varepsilon^2 R,$$

where $R \in \Psi^{-\infty}(\mathbb{R})$ (see (2-26)). As in the proof of Lemma 5.1, (6-4) follows from

$$\|(P_{\gamma,\varepsilon}(\alpha) - E')^{-1}\|_{L^2(\mathbb{R}) \to H_h^2(\mathbb{R})} \le 5/\varepsilon \tag{6-9}$$

for $E' \in [-E_0, E_0]$.

The proof of (6-9) combines elements of the proofs of (5-9) and (5-24). Let $\phi \in C_0^\infty(T^*\mathbb{R})$ be identically 1 near $\{0 \le r \le R_- + 1,\ |\rho| \le 2,\ |\operatorname{Re} p_\gamma| \le E_0\}$ and be supported such that $\operatorname{Re} H_{p_\gamma} q < 0$ on $\operatorname{supp}\phi$. Let Φ be the quantization of ϕ. For δ small enough, and h (and hence ε) small enough depending on δ, we have $|p_{\gamma,\varepsilon} - E'| \ge \delta(1+\rho^2)/C$ on $\operatorname{supp}(1-\phi)$, uniformly in $E' \in [-E_0, E_0]$, in $\alpha \le \alpha_0$ and in h, where $p_{\gamma,\varepsilon}(\alpha)$ is the semiclassical principal symbol of $P_{\gamma,\varepsilon}(\alpha)$. Hence, by the semiclassical elliptic estimate (2-18),

$$\|(\operatorname{Id} - \Phi)u\|_{H_h^2(\mathbb{R})} \le C\delta^{-1} \|(P_{\gamma,\varepsilon} - E')(\operatorname{Id} - \Phi)u\|_{L^2(\mathbb{R})} + \mathcal{O}(h^\infty)\|u\|_{H_h^{-N}(\mathbb{R})}.$$

Using (6-8) and $\operatorname{supp}\phi \subset \{\operatorname{Re} H_{p_c} q < 0\}$, fix C_q large enough that on $\operatorname{supp}\phi$ we have

$$\operatorname{Im} p_{\gamma,\varepsilon} = \operatorname{Im} p_\gamma + \varepsilon \operatorname{Re} H_{p_c} q \le -\alpha^2(1 - W_F)e^{-2(r + \operatorname{Re}\beta)}\gamma(1 + \mathcal{O}(\delta^2)) + \varepsilon \operatorname{Re} H_{p_c} q \le -\varepsilon.$$

Then, using the sharp Gårding inequality (2-19), we have, for h sufficiently small,

$$\begin{aligned} \|\Phi u\|_{L^2(\mathbb{R})} \|(P_{C,\varepsilon} - E')\Phi u\|_{L^2(\mathbb{R})} &\ge -\langle \operatorname{Im}(P_{C,\varepsilon} - E')\Phi u, \Phi u\rangle_{L^2(\mathbb{R})} \\ &\ge \varepsilon \|\Phi u\|_{L^2(\mathbb{R})}^2 - Ch\|u\|_{L^2(\mathbb{R})}^2. \end{aligned}$$

This implies (6-9) just as in the proofs of (5-9) and (5-24). □

Proof of (6-4) *for* $\alpha \ge \alpha_0$. Define contours $\gamma = \gamma_\alpha(r)$ as follows. Take R_α such that

$$\alpha^2 e^{-2R_\alpha} e^{2\max|\operatorname{Re}\beta|} = \min\{\tfrac14, \tfrac12 \tan\theta_0\}, \tag{6-10}$$

where $\max|\operatorname{Re}\beta|$ is taken over $\mathbb{R} \cup \{|z| > R_g,\ 0 \le \arg z \le \theta_0\}$. Note that $R_\alpha > R + 1$ by (6-7). Take γ smooth and supported in (R, ∞), with $0 \le \gamma'(r) \le \frac12$, and such that

$$\begin{cases} \gamma(r) \le \frac{\pi}{9}, & r \le R+1, \\ \frac{\pi}{18} \le \gamma(r) \le \frac{\pi}{6}, & R+1 \le r \le R_\alpha, \\ \gamma'(r) = \min\{\frac12, \tan\theta_0\}, & r \ge R_\alpha. \end{cases}$$

We prove that

$$|p_\gamma(\alpha) - E'| \geq (1+\rho^2)/C \tag{6-11}$$

uniformly for $-E \leq E' \leq E$ and $\alpha \geq \alpha_0$, by considering each range of r individually. By (2-18) this implies (6-4) for $\alpha \geq \alpha_0$.

(1) For $r \leq R+1$ we have

$$\begin{aligned} \operatorname{Re} p_\gamma(\alpha) + 1 &= \frac{\rho^2(1-\gamma'(r)^2)}{|1+i\gamma'(r)|^4} + \alpha^2(1-W_F(r)) \operatorname{Re} e^{-2(r+i\gamma(r)+\beta(r+i\gamma(r)))} \\ &\geq \tfrac{1}{3}\rho^2 + \alpha^2(1-W_F(r))e^{-2(r+\operatorname{Re}\beta(r+i\gamma(r)))}\cos(3\gamma(r)) \\ &\geq \tfrac{1}{3}\rho^2 + 4(1-W_F(r)), \end{aligned} \tag{6-12}$$

where for the first inequality we used $\gamma' \leq \frac{1}{2}$ and (6-6), and for the second (6-7) and $\gamma \leq \frac{\pi}{9}$. Since $\operatorname{Im} p_\gamma = -W_F$ whenever $W_F \neq 0$, this gives (6-11) for $r \leq R+1$.

(2) For $R+1 \leq r \leq R_\alpha$ we have $\operatorname{Re} p_\gamma(\alpha) \geq \frac{1}{3}\rho^2 - 1$ by the same argument as in (6-12). This gives (6-11) for $R+1 \leq r \leq R_\alpha$ once we note that (6-6) and (6-10) imply

$$\begin{aligned} -\operatorname{Im} p_\gamma(\alpha) &= \frac{2\rho^2\gamma'(r)}{|1+i\gamma'(r)|^4} - \alpha^2 \operatorname{Im} e^{-2(r+i\gamma(r)+\beta(r+i\gamma(r)))} \\ &\geq e^{-2\max|\operatorname{Re}\beta|}\sin\big(\tfrac{\pi}{18}\big)\min\big\{\tfrac{1}{2}, \tfrac{1}{2}\tan\theta_0\big\}. \end{aligned}$$

(3) For $r \geq R_\alpha$, note that $\alpha^2|e^{-2(r+i\gamma(r)+\beta(r+i\gamma(r)))}| \leq \gamma'(r)$. We again deduce (6-11) by considering two ranges of ρ individually. When $\rho^2/|1+i\gamma'(r)|^4 \leq \frac{1}{2}$ we have

$$\begin{aligned} \operatorname{Re} p_\gamma(\alpha) &= \frac{\rho^2(1-\gamma'(r)^2)}{|1+i\gamma'(r)|^4} + \alpha^2 \operatorname{Re} e^{-2(r+i\gamma(r)+\beta(r+i\gamma(r)))} - 1 \\ &\leq \tfrac{1}{2} + \tfrac{1}{4} - 1 = -\tfrac{1}{4}. \end{aligned}$$

When $\rho^2/|1+i\gamma'(r)|^4 \geq \frac{1}{2}$ we have

$$\begin{aligned} \operatorname{Im} p_\gamma(\alpha) &= \frac{-2\rho^2\gamma'(r)}{|1+i\gamma'(r)|^4} + \alpha^2 \operatorname{Im} e^{-2(r+i\gamma(r)+\beta(r+i\gamma(r)))} \\ &\leq \frac{-2\rho^2\gamma'(r)}{|1+i\gamma'(r)|^4} + \tfrac{1}{2}\gamma'(r) \leq -\tfrac{3}{2}\gamma'(r) = -\min\big\{\tfrac{3}{4}, \tfrac{3}{2}\tan\theta_0\big\}. \end{aligned}$$

□

For $\alpha \geq \alpha_0$, (6-5) follows from an Agmon estimate just as in the proof of (5-15) for $\alpha \geq \alpha_0$ above. For $\alpha \leq \alpha_0$, (6-5) follows from the same positive commutator argument as was used for the proof of (5-33).

7. Applications

In this section we give applications of the Theorem to solutions to Schrödinger and wave equations. Since such applications are well-known, we only sketch the arguments below, giving references to sources with further details.

We use the notation

$$\|u\|_s := \|(1+\Delta)^{s/2}u\|_{L^2(X)}, \quad \|A\|_{s\to s'} := \sup_{\|u\|_s=1} \|Au\|_{s'}, \quad s, s' \in \mathbb{R}.$$

We begin by using (1-1) to deduce polynomial bounds on the resolvent between Sobolev spaces. If $\chi, \tilde{\chi} \in C_0^\infty(X)$ satisfy $\tilde{\chi}\chi = \chi$, then for any $s \in \mathbb{R}$, we have

$$\|\Delta\chi u\|_s \le C(\|\tilde{\chi}u\|_s + \|\tilde{\chi}\Delta u\|_s).$$

Hence, for any $s, s' \in \mathbb{R}$, we have, letting $R_\chi(\sigma) := \chi\big(\Delta - \frac{1}{4}n^2 - \sigma^2\big)^{-1}\chi$,

$$\begin{aligned}\|R_\chi(\sigma)\|_{s\to s} &\le C\|R_{\tilde{\chi}}(\sigma)\|_{s'\to s'},\\ \|R_\chi(\sigma)\|_{s\to s'+2} &\le C(1+|\sigma|^2)\big(\|R_{\tilde{\chi}}(\sigma)\|_{s\to s} + \|R_{\tilde{\chi}}(\sigma)\|_{s\to s'}\big),\\ \|R_\chi(\sigma)\|_{s\to s'} &\le C(1+|\sigma|^2)^{-1}\big(\|R_{\tilde{\chi}}(\sigma)\|_{s\to s'+2} + \|R_{\tilde{\chi}}(\sigma)\|_{s\to s'}\big).\end{aligned}$$

Consequently, (1-1) implies that for any $\chi \in C_0^\infty(X)$, there is $M_0 > 0$ such that for any $M_1 > 0$, $s \in \mathbb{R}$, $s' \le s+2$, there is $M_2 > 0$ such that

$$\|R_\chi(\sigma)\|_{s\to s'} \le M_2|\sigma|^{M_0|\operatorname{Im}\sigma|+s'-s-1} \tag{7-1}$$

when $|\operatorname{Re}\sigma| \ge M_2$, $\operatorname{Im}\sigma \ge -M_1$.

7A. ***Local smoothing.*** By the self-adjoint functional calculus of Δ, the Schrödinger propagator is unitary on all Sobolev spaces: for any $s, t \in \mathbb{R}$, if $u \in H^s(X)$,

$$\|e^{-it\Delta}u\|_s = \|u\|_s.$$

The Kato local smoothing effect says that if we localize in space and average in time, then Sobolev regularity improves by half a derivative: for any $\chi \in C_0^\infty(X)$, $T > 0$, $s \in \mathbb{R}$ there is $C > 0$ such that if $u \in H^s(X)$,

$$\int_0^T \|\chi e^{-it\Delta}u\|_{s+1/2}^2\,dt \le C\|u\|_s^2. \tag{7-2}$$

This follows by a TT^* argument from (7-1) applied with $\operatorname{Im}\sigma = s = 0$, $s' = 1$ (see, e.g., [Burq 2004, p. 424]); note that in this case the right-hand side of (7-1) is independent of σ.

7B. ***Resonant wave expansions.*** Suppose $\chi\big(\Delta - \frac{1}{4}n^2 - \sigma^2\big)^{-1}\chi$ is meromorphic for $\sigma \in \mathbb{C}$. For example we may take (X, g) as in Section 2D1. More generally, if the funnel end is evenly asymptotically hyperbolic as in [Guillarmou 2005, Definition 1.2] then this follows as in the proof of Theorem 1.1 in [Sjöstrand and Zworski 1991, p. 747], but in the interest of brevity we do not pursue this here.

Then (7-1) implies that, when the initial data is compactly supported, solutions to the wave equation $\big(\partial_t^2 + \Delta - \frac{1}{4}n^2\big)u = 0$ can be expanded into a superposition of eigenstates and resonant states, with a remainder which decays exponentially on compact sets:

Let $\chi \in C_0^\infty(X)$. There is $M_0 > 0$ such that for any $s \in \mathbb{R}$, $f \in H^{s+1}(X)$, $g \in H^s(X)$ satisfying $\chi f = f$, $\chi g = g$, and for any $M_1 > 0$ and

$$s' < s - M_0 M_1, \tag{7-3}$$

there are $C, T > 0$ such that if $t \geq T$, $H = \sqrt{\Delta - \frac{1}{4}n^2}$, then

$$\left\| \chi \left(\cos(tH) f + \frac{\sin(tH)}{H} g - \sum_{\operatorname{Im}\sigma_j > -M_1} \sum_{m=1}^{M(\sigma_j)} e^{-i\sigma_j t} t^{m-1} w_{j,m} \right) \right\|_{s'} \leq C e^{-M_1 t},$$

where the sum is taken over poles of $R_\chi(\sigma)$ (and is finite by the Theorem), $M(\sigma_j)$ is the rank of the residue of the pole at σ_j, and each $w_{j,m}$ is a linear combination of the projections of f and g onto the m-th eigenstate or resonant state at σ_j. This follows from (7-1) by an argument of [Lax and Phillips 1989; Vaĭnberg 1989]; see also [Tang and Zworski 2000, Theorem 3.3] or [Datchev and Vasy 2012a, Corollary 6.1].

Remark. The local smoothing estimate (7-2) is lossless in the sense that the result is the same if (X, g) is nontrapping and asymptotically Euclidean or hyperbolic (see [Cardoso, Popov and Vodev 2004, (1.6)] for a general result). This is because the resolvent estimates (1-1) and (1-2) agree when $\operatorname{Im}\sigma = 0$. The resonant wave expansion exhibits a loss in the Sobolev spaces in which the remainder is controlled: the improvement from (1-1) to (1-2) for $\operatorname{Im}\sigma < 0$ means that, when (1-2) holds, we can replace (7-3) with $s' < s$.

8. Lower bounds

In this section we prove that, in the setting of an exact quotient, the holomorphic continuation of the resolvent grows polynomially. As in [Borthwick 2007, §5.3], we use the fact that in this case the integral kernel of the resolvent can be written in terms of modified Bessel functions.

Proposition 8.1. *Let* (X, g) *be given by*

$$X = \mathbb{R} \times S, \quad g = dr^2 + e^{2r} dS,$$

where (S, dS) *is a compact Riemannian manifold without boundary of dimension* n. *Then for any* $\chi \in C_0^\infty(X)$ *which is not identically* 0, *the cutoff resolvent* $\chi\left(\Delta - \frac{1}{4}n^2 - \sigma^2\right)^{-1}\chi$ *continues holomorphically from* $\{\operatorname{Im}\sigma > 0\}$ *to* $\mathbb{C} \setminus 0$, *with a simple pole of rank* 1 *at* $\sigma = 0$.

Moreover, if $\chi \neq 0$ *in a neighborhood of* $\{r = 0\}$, *for any* $\varepsilon > 0$ *there exists* $C > 0$ *such that*

$$\left\| \chi\left(\Delta - \tfrac{1}{4}n^2 - \sigma^2\right)^{-1} \chi \right\|_{L^2(X) \to L^2(X)} \geq e^{-C|\operatorname{Im}\sigma|} |\sigma|^{2|\operatorname{Im}\sigma| - 1} / C \tag{8-1}$$

when $\operatorname{Im}\sigma \leq -\varepsilon$, $\operatorname{Re}\sigma \geq C$, $|\operatorname{Im}\sigma| \leq C |\operatorname{Re}\sigma|^{2/3}$.

Proof. As in Section 2C a conjugation and separation of variables reduce this to the study of the following family of ordinary differential operators:

$$P_m = D_r^2 + \lambda_m^2 e^{-2r},$$

where $0 = \lambda_0 < \lambda_1 \le \lambda_2 \le \cdots$ are square roots of the eigenvalues of Δ. We will show that $\chi(P_m - \sigma^2)^{-1}\chi$ is entire in σ for $m > 0$, and that it is holomorphic in $\mathbb{C} \setminus 0$ with a simple pole of rank 1 at $\sigma = 0$ for $m = 0$. We will further show that

$$\|\chi(P_1 - \sigma^2)^{-1}\chi\|_{L^2(\mathbb{R}) \to L^2(\mathbb{R})} \ge e^{-C|\operatorname{Im}\sigma|}|\sigma|^{2|\operatorname{Im}\sigma|-1}/C \tag{8-2}$$

when $\operatorname{Im}\sigma \le -\varepsilon$, $\operatorname{Re}\sigma \ge C$, $|\operatorname{Im}\sigma| \le |\operatorname{Re}\sigma|^{2/3}$.

We write the integral kernel of the resolvent of each P_m using the following variation of parameters formula:

$$R_m(r, r') = -\psi_1(\max\{r, r'\})\psi_2(\min\{r, r'\})/W(\psi_1, \psi_2), \tag{8-3}$$

where ψ_1 and ψ_2 are linearly independent solutions to $(P_m - \sigma^2)u = 0$ and $W(\psi_1, \psi_2)$ is their Wronskian.

If $m = 0$ we take $\psi_1(r) = e^{ir\sigma}$ and $\psi_2(r) = e^{-ir\sigma}$ (this is the choice for which the resolvent maps L^2 to L^2 for $\operatorname{Im}\sigma > 0$), so that $W(\psi_1, \psi_2) = 2i\sigma$. Now the asserted continuation is immediate from the formula (8-3).

To study $m > 0$ we use, as in [Borthwick 2007, §5.3], the Bessel functions

$$\psi_1(r) = I_\nu(\lambda_m e^{-r}), \quad \psi_2(r) = K_\nu(\lambda_m e^{-r}), \quad \nu = -i\sigma. \tag{8-4}$$

We recall the definitions:

$$I_\nu(z) := \frac{z^\nu}{2^\nu}\sum_{k=0}^{\infty}\frac{(z/2)^{2k}}{k!\,\Gamma(\nu + k + 1)}, \tag{8-5}$$

$$K_\nu(z) := \frac{\pi}{2\sin(\pi\nu)}(I_{-\nu}(z) - I_\nu(z)). \tag{8-6}$$

This pair solves the desired equation (see for example [Olver 1974, Chapter 7, (8.01)]) and has Wronskian $W = 1$ (see for example [ibid., Chapter 7, (8.07)]). When $\operatorname{Im}\sigma > 0$, we have $\operatorname{Re}\nu > 0$ and this resolvent maps L^2 to L^2 thanks to the asymptotic

$$I_\nu(z) = \frac{z^\nu}{2^\nu\Gamma(\nu+1)}\Big(1 + \mathcal{O}\Big(\frac{z^2}{\nu}\Big)\Big), \tag{8-7}$$

which is a consequence of (8-5), and thanks to the fact that $K_\nu(z) \sim e^{-z}\sqrt{\pi/2z}$ as $z \to \infty$ (see for example [ibid., Chapter 7, (8.04)]). Because I and K are entire in ν, we have the desired holomorphic continuation of the resolvent for all $m > 0$.

To estimate the resolvent we use (8-6) and (8-7) to write

$$K_\nu(z) = \frac{\pi}{2\sin(\pi\nu)}\Big(\frac{z^{-\nu}}{2^{-\nu}\Gamma(-\nu+1)} - \frac{z^\nu}{2^\nu\Gamma(\nu+1)}\Big)\Big(1 + \mathcal{O}\Big(\frac{z^2}{\nu}\Big)\Big).$$

Using Euler's reflection formula for the gamma function (see for example [ibid., Chapter 2, (1.07)]),

$$\frac{\pi}{\sin(\pi\nu)\Gamma(\nu + 1)} = -\Gamma(-\nu) = \frac{\Gamma(-\nu + 1)}{\nu},$$

it follows that

$$K_\nu(z) = \frac{\Gamma(\nu+1)}{2\nu}\Big(\frac{z^{-\nu}}{2^{-\nu}} - \frac{z^\nu\Gamma(-\nu+1)}{2^\nu\Gamma(\nu+1)}\Big)\Big(1+\mathcal{O}\Big(\frac{z^2}{\nu}\Big)\Big)$$
$$= \frac{\Gamma(\nu+1)}{2\nu}\Big(\frac{z^{-\nu}}{2^{-\nu}} + \frac{\nu z^\nu \sin(\pi\nu)\Gamma(-\nu)^2}{2^\nu\pi}\Big)\Big(1+\mathcal{O}\Big(\frac{z^2}{\nu}\Big)\Big). \tag{8-8}$$

To prove (8-1) we assume (without loss of generality) that there is $a > 0$ such that $\chi \geq 1$ on $[-a, a]$, and fix such an a. Let f be the characteristic function of $[0, a]$, and let

$$u(r) := (P_1 - \sigma^2)^{-1} f(r) = -\int_0^a R_1(r, r')\, dr' = K_\nu(\lambda_1 e^{-r}) \int_0^a I_\nu(\lambda_1 e^{-r'})\, dr'.$$

Then $\|\chi(P_1-\sigma^2)^{-1}\chi\|_{L^2(\mathbb{R})\to L^2(\mathbb{R})} \geq \|\chi u\|_{L^2(\mathbb{R})}/\|f\|_{L^2(\mathbb{R})}$ and hence

$$\|\chi(P_1-\sigma^2)^{-1}\chi\|^2_{L^2(\mathbb{R})\to L^2(\mathbb{R})} \geq \frac{1}{a}\int_{-a}^a |u(r)|^2\, dr \geq \frac{1}{a}\int_{-a}^0 \Big| K_\nu(\lambda_1 e^{-r}) \int_0^a I_\nu(\lambda_1 e^{-r'})\, dr'\Big|^2\, dr$$
$$= \frac{1}{a}\Big|\int_0^a I_\nu(\lambda_1 e^{-r'})\, dr'\Big|^2 \int_{-a}^0 |K_\nu(\lambda_1 e^{-r})|^2\, dr.$$

Using (8-7) and (8-8) we obtain

$$\|\chi(P_1-\sigma^2)^{-1}\chi\|^2_{L^2(\mathbb{R})\to L^2(\mathbb{R})}$$
$$\geq \frac{1}{8a|\nu|^2}\Big|\int_0^a \frac{(\lambda_1 e^{-r'})^\nu}{2^\nu}\, dr'\Big|^2 \int_{-a}^0 \Big|\frac{(\lambda_1 e^{-r})^{-\nu}}{2^{-\nu}} + \frac{\nu(\lambda_1 e^{-r})^\nu \sin(\pi\nu)\Gamma(-\nu)^2}{2^\nu\pi}\Big|^2\, dr, \tag{8-9}$$

provided $|\nu|$ is sufficiently large.

We now bound the two integrals from below one by one. First,

$$\Big|\int_0^a \frac{(\lambda_1 e^{-r'})^\nu}{2^\nu} dr'\Big| = \frac{\lambda_1^{\operatorname{Re}\nu}}{2^{\operatorname{Re}\nu}|\nu|}|e^{-a\nu} - 1| \geq e^{-C|\operatorname{Re}\nu|}/C|\nu|, \tag{8-10}$$

since $\operatorname{Re}\nu = \operatorname{Im}\sigma \leq -\varepsilon$. Second, using Stirling's formula (see for example [ibid., Chapter 8, (4.04)])

$$\Gamma(-\nu) = e^\nu(-\nu)^{-\nu}\sqrt{-2\pi/\nu}(1+\mathcal{O}(\nu^{-1})),$$

with

$$\arg(-\nu) := \frac{\pi}{2} - \arctan\frac{|\operatorname{Re}\nu|}{|\operatorname{Im}\nu|}$$

taking values in $\big(0, \frac{\pi}{2}\big)$, and where the branch of $(-\nu)^{-\nu}$ is real and positive when $-\nu$ is, we write

$$|\nu\sin(\pi\nu)\Gamma(-\nu)^2| = \pi e^{\pi|\operatorname{Im}\nu|}e^{-2|\operatorname{Re}\nu|}|\nu|^{2|\operatorname{Re}\nu|}e^{-2|\operatorname{Im}\nu|\arg(-\nu)}(1+\mathcal{O}(|\operatorname{Im}\nu|^{-1})),$$
$$= \pi e^{-2|\operatorname{Re}\nu|}|\nu|^{2|\operatorname{Re}\nu|}e^{2|\operatorname{Im}\nu|\arctan|\operatorname{Re}\nu/\operatorname{Im}\nu|}(1+\mathcal{O}(|\operatorname{Im}\nu|^{-1}))$$
$$= \pi|\nu|^{2|\operatorname{Re}\nu|}e^{-\frac{2}{3}|\operatorname{Re}\nu|^3/|\operatorname{Im}\nu|^2}(1+\mathcal{O}(|\operatorname{Re}\nu|^5|\operatorname{Im}\nu|^{-4}+|\operatorname{Im}\nu|^{-1})).$$

Hence, as long as $|\mathrm{Re}\,\nu|^{-3}|\mathrm{Im}\,\nu|^2$ is bounded and $|\nu|$ is sufficiently large, and using $\mathrm{Re}\,\nu \le -\varepsilon$,

$$\left|\frac{(\lambda_1 e^{-r})^{-\nu}}{2^{-\nu}} + \frac{\nu(\lambda_1 e^{-r})^{\nu}\sin(\pi\nu)\Gamma(-\nu)^2}{2^{\nu}\pi}\right| \ge \tfrac{1}{2}|\nu|^{-2\,\mathrm{Re}\,\nu} e^{\frac{2}{3}(\mathrm{Re}\,\nu)^3/(\mathrm{Im}\,\nu)^2}\frac{(\lambda_1 e^{-r})^{\mathrm{Re}\,\nu}}{2^{\mathrm{Re}\,\nu}} - \frac{2^{\mathrm{Re}\,\nu}}{(\lambda_1 e^{-r})^{\mathrm{Re}\,\nu}}$$
$$\ge \frac{1}{C}|\nu|^{2|\mathrm{Re}\,\nu|}\left(\frac{2e^r}{\lambda_1}\right)^{|\mathrm{Re}\,\nu|}$$

for $|r| \le a$. This implies

$$\int_a^0 \left|\frac{(\lambda_1 e^{-r})^{-\nu}}{2^{-\nu}} + \frac{\nu(\lambda_1 e^{-r})^{\nu}\sin(\pi\nu)\Gamma(-\nu)^2}{2^{\nu}\pi}\right|^2 dr \ge \frac{1}{C}|\nu|^{4|\mathrm{Re}\,\nu|}\left(\frac{2}{\lambda_1}\right)^{2|\mathrm{Re}\,\nu|}\int_{-a}^0 e^{2|\mathrm{Re}\,\nu| r}\,dr$$
$$\ge |\nu|^{4|\mathrm{Re}\,\nu|}e^{-C\,\mathrm{Re}\,\nu}/C.$$

Combining this with (8-9) and (8-10), and using $\nu = -i\sigma$, gives (8-2) and hence (8-1). □

Appendix: The curvature of a warped product

The result of this calculation is used in the examples in Section 2D, and although it is well known, we include the details for the convenience of the reader. For this section only, let $(S, \tilde{g})$ be a compact Riemannian manifold, and let $X = \mathbb{R} \times S$ have the metric

$$g = dr^2 + f(r)^2\tilde{g},$$

where $f \in C^\infty(\mathbb{R}; (0,\infty))$. Let $p \in X$, let P be a two-dimensional subspace of T_pX, and let $K(P)$ be the sectional curvature of P with respect to g. We will show that if $\partial_r \in P$, then

$$K(P) = -f''(r)/f(r),$$

while if $P \subset T_pS$ and $\widetilde{K}(P)$ is the sectional curvature of P with respect to $\tilde{g}$, then

$$K(P) = (\widetilde{K}(P) - f'(r)^2)/f(r)^2.$$

We work in coordinates $(x^0, \dots, x^n) = (r, x^1, \dots, x^n)$, and write

$$g = g_{\alpha\beta}\,dx^\alpha\,dx^\beta = dr^2 + g_{ij}\,dx^i\,dx^j = dr^2 + f(r)^2\tilde{g}_{ij}\,dx^i\,dx^j,$$

using the Einstein summation convention. We use Greek letters for indices which include 0, that is indices which include r, and Latin letters for indices which do not. Then

$$\partial_\alpha g_{r\alpha} = 0, \quad \partial_r g_{jk} = 2f^{-1}f'g_{jk}, \quad \partial_i g_{jk} = f^2\partial_i\tilde{g}_{jk}.$$

We write Γ for the Christoffel symbols of g, and $\widetilde{\Gamma}$ for those of $\tilde{g}$. These are given by

$$\Gamma^r{}_{r\alpha} = \Gamma^\alpha{}_{rr} = 0, \quad \Gamma^r{}_{jk} = -f^{-1}f'g_{jk}, \quad \Gamma^i{}_{jr} = f^{-1}f'\delta^i_j, \quad \Gamma^i{}_{jk} = \widetilde{\Gamma}^i{}_{jk}.$$

Let R be the Riemann curvature tensor of g:

$$R_{\alpha\beta\gamma}{}^\delta = \partial_\alpha\Gamma^\delta{}_{\beta\gamma} + \Gamma^\varepsilon{}_{\beta\gamma}\Gamma^\delta{}_{\alpha\varepsilon} - \partial_\beta\Gamma^\delta{}_{\alpha\gamma} - \Gamma^\varepsilon{}_{\alpha\gamma}\Gamma^\delta{}_{\beta\varepsilon}.$$

Now if $P \subset T_pX$ is spanned by a pair of orthogonal unit vectors $V^\alpha\partial_\alpha$ and $W^\alpha\partial_\alpha$, then $K(P) = R_{\alpha\beta\gamma\delta}V^\alpha W^\beta W^\gamma V^\delta$, and similarly for $\widetilde{R}$ and $\widetilde{K}$. Then

$$R_{ijk}{}^l = \widetilde{R}_{ijk}{}^l + \Gamma^r{}_{jk}\Gamma^l{}_{ir} - \Gamma^r{}_{ik}\Gamma^l{}_{jr} = \widetilde{R}_{ijk}{}^l + (f^{-1})^2(f')^2(-\delta_i^l g_{jk} + \delta_j^l g_{ik}),$$
$$R_{rjk}{}^r = \partial_r\Gamma^r{}_{jk} - \Gamma^m{}_{rk}\Gamma^r{}_{jm} = -(f^{-1}f'g_{jk})' + (f^{-1}f')^2 g_{jk} = -f^{-1}f''g_{jk}.$$

If $\partial_r \in P$ we take $V = \partial_r$ and $W = W^j\partial_j$ any unit vector in T_pX orthogonal to V. Then

$$K(P) = R_{rjkr}W^jW^k = -f^{-1}f''g_{jk}W^jW^k = -f^{-1}f''.$$

Meanwhile, if $\partial_r \perp P$, we may write $V = V^j\partial_j$ and $W = W^j\partial_j$. Then

$$K(P) = \big(f^2\tilde{R}_{ijkl} + (f^{-1})^2(f')^2(-g_{li}g_{jk} + g_{lj}g_{ik})\big)V^iW^jW^kV^l.$$

Using the fact that fV and fW are orthogonal unit vectors for $\tilde{g}$, we see that

$$K(P) = f^{-2}\tilde{K}(P) - (f^{-1})^2(f')^2.$$

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References

[Aguilar and Combes 1971] J. Aguilar and J. M. Combes, "A class of analytic perturbations for one-body Schrödinger Hamiltonians", *Comm. Math. Phys.* **22** (1971), 269–279. MR 0345551 Zbl 0219.47011

[Alexandrova and Tamura 2011] I. Alexandrova and H. Tamura, "Resonance free regions in magnetic scattering by two solenoidal fields at large separation", *J. Funct. Anal.* **260**:6 (2011), 1836–1885. MR 2754895 Zbl 1211.81093

[Baskin and Wunsch 2013] D. Baskin and J. Wunsch, "Resolvent estimates and local decay of waves on conic manifolds", *J. Differential Geom.* **95**:2 (2013), 183–214. MR 3128982 Zbl 1296.53075

[Bony and Häfner 2008] J.-F. Bony and D. Häfner, "Decay and non-decay of the local energy for the wave equation on the de Sitter–Schwarzschild metric", *Comm. Math. Phys.* **282**:3 (2008), 697–719. MR 2426141 Zbl 1159.35007

[Bony and Petkov 2013] J.-F. Bony and V. Petkov, "Semiclassical estimates of the cut-off resolvent for trapping perturbations", *J. Spectr. Theory* **3**:3 (2013), 399–422. MR 3073417 Zbl 1290.47013

[Borthwick 2007] D. Borthwick, *Spectral theory of infinite-area hyperbolic surfaces*, Progress in Mathematics **256**, Birkhäuser, Boston, 2007. MR 2344504 Zbl 1130.58001

[Bridson and Haefliger 1999] M. R. Bridson and A. Haefliger, *Metric spaces of non-positive curvature*, Grundlehren der Math. Wissenschaften **319**, Springer, Berlin, 1999. MR 1744486 Zbl 0988.53001

[Burq 1998] N. Burq, "Décroissance de l'énergie locale de l'équation des ondes pour le problème extérieur et absence de résonance au voisinage du réel", *Acta Math.* **180**:1 (1998), 1–29. MR 1618254 Zbl 0918.35081

[Burq 2002] N. Burq, "Lower bounds for shape resonances widths of long range Schrödinger operators", *Amer. J. Math.* **124**:4 (2002), 677–735. MR 1914456 Zbl 1013.35019

[Burq 2004] N. Burq, "Smoothing effect for Schrödinger boundary value problems", *Duke Math. J.* **123**:2 (2004), 403–427. MR 2066943 Zbl 1061.35024

[Burq and Zworski 2004] N. Burq and M. Zworski, "Geometric control in the presence of a black box", *J. Amer. Math. Soc.* **17**:2 (2004), 443–471. MR 2051618 Zbl 1050.35058

[Burq, Guillarmou and Hassell 2010] N. Burq, C. Guillarmou, and A. Hassell, "Strichartz estimates without loss on manifolds with hyperbolic trapped geodesics", *Geom. Funct. Anal.* **20**:3 (2010), 627–656. MR 2720226 Zbl 1206.58009

[Cardoso and Vodev 2002] F. Cardoso and G. Vodev, "Uniform estimates of the resolvent of the Laplace–Beltrami operator on infinite volume Riemannian manifolds, II", *Ann. Henri Poincaré* **3**:4 (2002), 673–691. MR 1933365 Zbl 1021.58016

[Cardoso, Popov and Vodev 2004] F. Cardoso, G. Popov, and G. Vodev, "Semi-classical resolvent estimates for the Schrödinger operator on non-compact complete Riemannian manifolds", *Bull. Braz. Math. Soc.* (*N.S.*) **35**:3 (2004), 333–344. MR 2106308 Zbl 1159.58308

[Christianson 2009] H. Christianson, "Applications of cutoff resolvent estimates to the wave equation", *Math. Res. Lett.* **16**:4 (2009), 577–590. MR 2525026 Zbl 1189.58012

[Christianson, Schenck, Vasy and Wunsch 2014] H. Christianson, E. Schenck, A. Vasy, and J. Wunsch, "From resolvent estimates to damped waves", *J. Anal. Math.* **122** (2014), 143–162. MR 3183526 Zbl 1301.35191

[Datchev 2010] K. Datchev, *Distribution of resonances for manifolds with hyperbolic ends*, Ph.D. thesis, University of California, Berkeley, 2010, available at http://search.proquest.com/docview/748836620.

[Datchev 2012] K. Datchev, "Extending cutoff resolvent estimates via propagation of singularities", *Comm. Partial Differential Equations* **37**:8 (2012), 1456–1461. MR 2957548 Zbl 1254.35034

[Datchev and Dyatlov 2013] K. Datchev and S. Dyatlov, "Fractal Weyl laws for asymptotically hyperbolic manifolds", *Geom. Funct. Anal.* **23**:4 (2013), 1145–1206. MR 3077910 Zbl 1297.58006

[Datchev and Vasy 2012a] K. Datchev and A. Vasy, "Gluing semiclassical resolvent estimates via propagation of singularities", *Int. Math. Res. Not.* **2012**:23 (2012), 5409–5443. MR 2999147 Zbl 1262.58019

[Datchev and Vasy 2012b] K. Datchev and A. Vasy, "Propagation through trapped sets and semiclassical resolvent estimates", *Ann. Inst. Fourier* (*Grenoble*) **62**:6 (2012), 2347–2377. MR 3060760 Zbl 1271.58014

[Datchev, Kang and Kessler 2015] K. R. Datchev, D. D. Kang, and A. P. Kessler, "Non-trapping surfaces of revolution with long-living resonances", *Math. Res. Lett.* **22**:1 (2015), 23–42. MR 3342177 Zbl 1328.58028

[Dimassi and Sjöstrand 1999] M. Dimassi and J. Sjöstrand, *Spectral asymptotics in the semi-classical limit*, London Mathematical Society Lecture Note Series **268**, Cambridge University Press, 1999. MR 1735654 Zbl 0926.35002

[Dyatlov 2012] S. Dyatlov, "Asymptotic distribution of quasi-normal modes for Kerr–de Sitter black holes", *Ann. Henri Poincaré* **13**:5 (2012), 1101–1166. MR 2935116 Zbl 1246.83111

[Dyatlov 2015a] S. Dyatlov, "Asymptotics of linear waves and resonances with applications to black holes", *Comm. Math. Phys.* **335**:3 (2015), 1445–1485. MR 3320319 Zbl 1315.83022

[Dyatlov 2015b] S. Dyatlov, "Resonance projectors and asymptotics for r-normally hyperbolic trapped sets", *J. Amer. Math. Soc.* **28**:2 (2015), 311–381. MR 3300697 Zbl 06394348

[Dyatlov and Zahl 2015] S. Dyatlov and J. Zahl, "Spectral gaps, additive energy, and a fractal uncertainty principle", preprint, 2015. arXiv 1504.06589

[Dyatlov and Zworski 2016] S. Dyatlov and M. Zworski, "Mathematical theory of scattering resonances", book project in progress, 2016, available at http://math.mit.edu/∼dyatlov/res/.

[Galkowski 2015] J. Galkowski, "Distribution of resonances in scattering by thin barriers", preprint, 2015. arXiv 1404.3709

[Galkowski 2016] J. Galkowski, "A quantitative Vainberg method for black box scattering", preprint, 2016. To appear in Comm. Math. Phys. arXiv 1511.05894

[Galkowski and Smith 2015] J. Galkowski and H. F. Smith, "Restriction bounds for the free resolvent and resonances in lossy scattering", *Int. Math. Res. Not.* **2015**:16 (2015), 7473–7509. MR 3428971 Zbl 06486428

[Guillarmou 2005] C. Guillarmou, "Meromorphic properties of the resolvent on asymptotically hyperbolic manifolds", *Duke Math. J.* **129**:1 (2005), 1–37. MR 2153454 Zbl 1099.58011

[Guillarmou and Mazzeo 2012] C. Guillarmou and R. Mazzeo, "Resolvent of the Laplacian on geometrically finite hyperbolic manifolds", *Invent. Math.* **187**:1 (2012), 99–144. MR 2874936 Zbl 1252.58015

[Guillarmou and Naud 2009] C. Guillarmou and F. Naud, "Wave decay on convex co-compact hyperbolic manifolds", *Comm. Math. Phys.* **287**:2 (2009), 489–511. MR 2481747 Zbl 1196.58011

[Guillopé and Zworski 1997] L. Guillopé and M. Zworski, "Scattering asymptotics for Riemann surfaces", *Ann. of Math.* (2) **145**:3 (1997), 597–660. MR 1454705 Zbl 0898.58054

[Guillopé, Lin and Zworski 2004] L. Guillopé, K. K. Lin, and M. Zworski, "The Selberg zeta function for convex co-compact Schottky groups", *Comm. Math. Phys.* **245**:1 (2004), 149–176. MR 2036371 Zbl 1075.11059

[Ikawa 1982] M. Ikawa, "Decay of solutions of the wave equation in the exterior of two convex obstacles", *Osaka J. Math.* **19**:3 (1982), 459–509. MR 676233 Zbl 0498.35008

[Lax and Phillips 1989] P. D. Lax and R. S. Phillips, *Scattering theory*, 2nd ed., Pure and Applied Mathematics **26**, Academic Press, Boston, 1989. MR 1037774 Zbl 0697.35004

[Martinez 2002] A. Martinez, "Resonance free domains for non globally analytic potentials", *Ann. Henri Poincaré* **3**:4 (2002), 739–756. Erratum published in *Ann. Henri Poincaré* **8**:7 (2007), 1425–1431. MR 1933368 Zbl 1026.81012

[Mazzeo and Melrose 1987] R. R. Mazzeo and R. B. Melrose, "Meromorphic extension of the resolvent on complete spaces with asymptotically constant negative curvature", *J. Funct. Anal.* **75**:2 (1987), 260–310. MR 916753 Zbl 0636.58034

[Melrose and Sjöstrand 1982] R. B. Melrose and J. Sjöstrand, "Singularities of boundary value problems, II", *Comm. Pure Appl. Math.* **35**:2 (1982), 129–168. MR 644020 Zbl 0546.35083

[Melrose, Sá Barreto and Vasy 2014] R. Melrose, A. Sá Barreto, and A. Vasy, "Asymptotics of solutions of the wave equation on de Sitter–Schwarzschild space", *Comm. Partial Differential Equations* **39**:3 (2014), 512–529. MR 3169793 Zbl 1286.35145

[Morawetz, Ralston and Strauss 1977] C. S. Morawetz, J. V. Ralston, and W. A. Strauss, "Decay of solutions of the wave equation outside nontrapping obstacles", *Comm. Pure Appl. Math.* **30**:4 (1977), 447–508. MR 0509770 Zbl 0372.35008

[Nakamura, Stefanov and Zworski 2003] S. Nakamura, P. Stefanov, and M. Zworski, "Resonance expansions of propagators in the presence of potential barriers", *J. Funct. Anal.* **205**:1 (2003), 180–205. MR 2020213 Zbl 1037.35064

[Nonnenmacher and Zworski 2009] S. Nonnenmacher and M. Zworski, "Quantum decay rates in chaotic scattering", *Acta Math.* **203**:2 (2009), 149–233. MR 2570070 Zbl 1226.35061

[Nonnenmacher and Zworski 2015] S. Nonnenmacher and M. Zworski, "Decay of correlations for normally hyperbolic trapping", *Invent. Math.* **200**:2 (2015), 345–438. MR 3338007 Zbl 06442708

[Olver 1974] F. W. J. Olver, *Asymptotics and special functions*, Academic Press, New York, 1974. MR 0435697 Zbl 0303.41035

[Petkov and Stoyanov 2010] V. Petkov and L. Stoyanov, "Analytic continuation of the resolvent of the Laplacian and the dynamical zeta function", *Anal. PDE* **3**:4 (2010), 427–489. MR 2718260 Zbl 1251.37031

[Reed and Simon 1978] M. Reed and B. Simon, *Methods of modern mathematical physics, IV: Analysis of operators*, Academic Press, New York, 1978. MR 0493421 Zbl 0401.47001

[Regge 1958] T. Regge, "Analytic properties of the scattering matrix", *Nuovo Cimento* (10) **8** (1958), 671–679. MR 0095702 Zbl 0080.41903

[Sá Barreto and Wang 2015] A. Sá Barreto and Y. Wang, "High energy resolvent estimates on conformally compact manifolds with variable curvature at infinity", preprint, 2015. arXiv 1511.05891

[Selberg 1990] A. Selberg, "Remarks on the distribution of poles of Eisenstein series", pp. 251–278 in *Festschrift in honor of I. I. Piatetski-Shapiro on the occasion of his sixtieth birthday, Part II* (Ramat Aviv, 1989), edited by S. Gelbart et al., Israel Math. Conf. Proc. **3**, Weizmann, Jerusalem, 1990. MR 1159119 Zbl 0712.11034

[Simon 1972] B. Simon, "Quadratic form techniques and the Balslev–Combes theorem", *Comm. Math. Phys.* **27** (1972), 1–9. MR 0321456 Zbl 0237.35025

[Sjöstrand 1990] J. Sjöstrand, "Geometric bounds on the density of resonances for semiclassical problems", *Duke Math. J.* **60**:1 (1990), 1–57. MR 1047116 Zbl 0702.35188

[Sjöstrand and Zworski 1991] J. Sjöstrand and M. Zworski, "Complex scaling and the distribution of scattering poles", *J. Amer. Math. Soc.* **4**:4 (1991), 729–769. MR 1115789 Zbl 0752.35046

[Sjöstrand and Zworski 2007] J. Sjöstrand and M. Zworski, "Fractal upper bounds on the density of semiclassical resonances", *Duke Math. J.* **137**:3 (2007), 381–459. MR 2309150 Zbl 1201.35189

[Tang and Zworski 1998] S.-H. Tang and M. Zworski, "From quasimodes to resonances", *Math. Res. Lett.* **5**:3 (1998), 261–272. MR 1637824 Zbl 0913.35101

[Tang and Zworski 2000] S.-H. Tang and M. Zworski, "Resonance expansions of scattered waves", *Comm. Pure Appl. Math.* **53**:10 (2000), 1305–1334. MR 1768812 Zbl 1032.35148

[Vaĭnberg 1989] B. R. Vaĭnberg, *Asymptotic methods in equations of mathematical physics*, Gordon & Breach, New York, 1989. MR 1054376 Zbl 0743.35001

[Vasy 2013] A. Vasy, "Microlocal analysis of asymptotically hyperbolic and Kerr–de Sitter spaces", *Invent. Math.* **194**:2 (2013), 381–513. MR 3117526 Zbl 1315.35015

[Vasy and Zworski 2000] A. Vasy and M. Zworski, "Semiclassical estimates in asymptotically Euclidean scattering", *Comm. Math. Phys.* **212**:1 (2000), 205–217. MR 1764368 Zbl 0955.58023

[Wang 2014] Y. Wang, "Resolvent and radiation fields on non-trapping asymptotically hyperbolic manifolds", preprint, 2014. arXiv 1410.6936

[Wunsch 2012] J. Wunsch, "Resolvent estimates with mild trapping", pp. Exposé 13 in *Journées équations aux dérivées partielles* (Biarritz, France, 2012), Cedram, 2012.

[Wunsch and Zworski 2011] J. Wunsch and M. Zworski, "Resolvent estimates for normally hyperbolic trapped sets", *Ann. Henri Poincaré* **12**:7 (2011), 1349–1385. MR 2846671 Zbl 1228.81170

[Zworski 1987] M. Zworski, "Distribution of poles for scattering on the real line", *J. Funct. Anal.* **73**:2 (1987), 277–296. MR 899652 Zbl 0662.34033

[Zworski 1999] M. Zworski, "Dimension of the limit set and the density of resonances for convex co-compact hyperbolic surfaces", *Invent. Math.* **136**:2 (1999), 353–409. MR 1688441 Zbl 1016.58014

[Zworski 2012] M. Zworski, *Semiclassical analysis*, Graduate Studies in Mathematics **138**, American Mathematical Society, Providence, RI, 2012. MR 2952218 Zbl 1252.58001

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CHARACTERIZING REGULARITY OF DOMAINS VIA THE RIESZ TRANSFORMS ON THEIR BOUNDARIES

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Under mild geometric measure-theoretic assumptions on an open subset Ω of $\mathbb{R}^n$, we show that the Riesz transforms on its boundary are continuous mappings on the Hölder space $\mathscr{C}^\alpha(\partial\Omega)$ if and only if Ω is a Lyapunov domain of order α (i.e., a domain of class $\mathscr{C}^{1+\alpha}$). In the category of Lyapunov domains we also establish the boundedness on Hölder spaces of singular integral operators with kernels of the form $P(x-y)/|x-y|^{n-1+l}$, where P is any odd homogeneous polynomial of degree l in $\mathbb{R}^n$. This family of singular integral operators, which may be thought of as generalized Riesz transforms, includes the boundary layer potentials associated with basic PDEs of mathematical physics, such as the Laplacian, the Lamé system, and the Stokes system. We also consider the limiting case $\alpha = 0$ (with VMO($\partial\Omega$) as the natural replacement of $\mathscr{C}^\alpha(\partial\Omega)$), and discuss an extension to the scale of Besov spaces.

1. Introduction

Let $\Omega \subset \mathbb{R}^n$ be an open set. Singular integral operators mapping functions on $\partial\Omega$ into functions defined either on $\partial\Omega$ or in Ω arise naturally in many branches of mathematics and engineering. From the work of G. David and S. Semmes [1991; 1993] we know that uniformly rectifiable (UR) sets make up the most general context in which Calderón–Zygmund-like operators are bounded on Lebesgue spaces L^p, with $p \in (1, \infty)$ (see Theorem 3.1 in the body of the paper for a concrete illustration of the scope of this theory). David and Semmes have also proved that, under the background assumption of Ahlfors regularity, uniform rectifiability is implied by the simultaneous L^2-boundedness of all integral convolution-type operators on $\partial\Omega$, whose kernels are smooth, odd, and satisfy standard growth conditions (see [David and Semmes 1993, Definition 1.20, p. 11]). In fact, a remarkable recent result proved by F. Nazarov, X. Tolsa,

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and A. Volberg [Nazarov et al. 2014] states that the L^2-boundedness of the Riesz transforms alone yields uniform rectifiability. The corresponding result in the plane was proved much earlier in [Mattila et al. 1996].

The above discussion points to uniform rectifiability as being intimately connected with the boundedness of a large class of Calderón–Zygmund-like operators on Lebesgue spaces. This being said, uniform rectifiability is far too weak to guarantee, by itself, analogous boundedness properties in other functional analytic contexts, such as the scale of Hölder spaces $\mathscr{C}^\alpha$, with $\alpha \in (0, 1)$.

The goal of this paper is to identify the category of domains for which the Riesz transforms are bounded on Hölder spaces as the class of Lyapunov domains (see Definition 2.1), and also show that, in fact, a much larger family of singular integral operators (generalizing the Riesz transforms) act naturally in this setting. On this note we wish to remark that the trademark property of Lyapunov domains is the Hölder continuity of their outward unit normals. Alternative characterizations, of a purely geometric flavor, may be found in [Alvarado et al. 2011]. The issue of boundedness of singular integral operators on Hölder spaces has a long history, with early work focused on Cauchy-type operators in the plane (see [Muskhelishvili 1953; Gakhov 1966], and the references therein). More recently this topic has been considered in [Dyn′kin 1979; 1980; Fabes et al. 1999; García-Cuerva and Gatto 2005; Gatto 2009; Kress 1989; Mateu et al. 2009; Meyer 1990, Chapter X, §4; Taylor 2000; Wittmann 1987].

Consider an Ahlfors regular subset Σ of $\mathbb{R}^n$ (i.e., a closed, nonempty set satisfying (2-21)), and equip it with $\mathcal{H}^{n-1}$, the $(n-1)$-dimensional Hausdorff measure in $\mathbb{R}^n$ restricted to Σ. The latter measure happens to be a positive, locally finite, complete, doubling, Borel regular (hence Radon) measure on Σ. In particular, the Lebesgue scale $L^p(\Sigma)$, $0 < p \leq \infty$, is always understood with respect to the aforementioned measure. A good deal of analysis goes through in this setting, such as the L^p-boundedness of the Hardy–Littlewood maximal operator on Σ, Lebesgue's differentiation theorem for locally integrable functions on Σ, and the density of Hölder functions with bounded support in $L^p(\Sigma)$. See, e.g., [Alvarado and Mitrea 2015; Coifman and Weiss 1971; 1977; Christ 1990], and the references therein.

Classically, given an Ahlfors regular subset Σ of $\mathbb{R}^n$, the Riesz transforms are defined as principal value singular integral operators on Σ with kernels $(x_j - y_j)/(\omega_{n-1}|x-y|^n)$ for $1 \leq j \leq n$. Specifically, if ω_{n-1} is the area of the unit sphere in $\mathbb{R}^n$, for each $j \in \{1, \dots, n\}$ define the j-th principal value Riesz transform

$$R_j^{\mathrm{pv}} f(x) := \lim_{\varepsilon \to 0^+} R_{j,\varepsilon} f(x), \tag{1-1}$$

where, for each $\varepsilon > 0$,

$$R_{j,\varepsilon} f(x) := \frac{1}{\omega_{n-1}} \int_{\substack{y \in \Sigma \\ |x-y|>\varepsilon}} \frac{x_j - y_j}{|x-y|^n} f(y)\, d\mathcal{H}^{n-1}(y), \qquad x \in \Sigma. \tag{1-2}$$

It turns out that if Σ is countably rectifiable (of dimension $n-1$) then for each $f \in L^2(\Sigma)$ the above limit exists at $\mathcal{H}^{n-1}$-a.e. point $x \in \Sigma$. In fact, a result of Tolsa [2008] states that if an arbitrary set $\Sigma \subset \mathbb{R}^n$ has $\mathcal{H}^{n-1}(\Sigma) < +\infty$ then:

Σ is countably rectifiable (of dimension $n-1$) if and only if, for each $j \in \{1, \dots, n\}$,

$$\lim_{\varepsilon \to 0^+} \int_{\substack{y \in \Sigma \\ |y-x|>\varepsilon}} \frac{x_j - y_j}{|x-y|^n} \, d\mathcal{H}^{n-1}(y) \tag{1-3}$$

exists for $\mathcal{H}^{n-1}$-a.e. point x belonging to Σ.

There is yet another related brand of Riesz transforms whose definition places no additional demands on the underlying Ahlfors regular set Σ of $\mathbb{R}^n$. The definition in question is of a distribution theory flavor and proceeds by fixing $\alpha \in (0, 1)$ and considering $\mathscr{C}^\alpha_c(\Sigma)$, the space of Hölder functions of order α with compact support in Σ. This is a Banach space, and we denote by $(\mathscr{C}^\alpha_c(\Sigma))^*$ its dual. Then, for each $j \in \{1, \dots, n\}$, one defines the j-th distributional Riesz transform as the operator

$$R_j : \mathscr{C}^\alpha_c(\Sigma) \longrightarrow (\mathscr{C}^\alpha_c(\Sigma))^* \tag{1-4}$$

with the property that for every $f, g \in \mathscr{C}^\alpha_c(\Sigma)$ one has

$$\langle R_j f, g \rangle = \frac{1}{2\omega_{n-1}} \int_\Sigma \int_\Sigma \frac{x_j - y_j}{|x-y|^n} [f(y)g(x) - f(x)g(y)] \, d\mathcal{H}^{n-1}(y) \, d\mathcal{H}^{n-1}(x), \tag{1-5}$$

where, in this context, $\langle \cdot, \cdot \rangle$ stands for the natural pairing between $(\mathscr{C}^\alpha_c(\Sigma))^*$ and $\mathscr{C}^\alpha_c(\Sigma)$. It may be checked without difficulty that the above integral is absolutely convergent, ultimately rendering the distributional Riesz transform R_j linear and continuous in the context of (1-4). Moreover, the distributional Riesz transform R_j just introduced is associated with the kernel $(x_j - y_j)/(\omega_{n-1}|x-y|^n)$ in the sense that, for each $f \in \mathscr{C}^\alpha_c(\Sigma)$, the functional $R_j f \in (\mathscr{C}^\alpha_c(\Sigma))^*$ is of function type on the set $\Sigma \setminus \operatorname{supp} f$ and

$$R_j f(x) = \frac{1}{\omega_{n-1}} \int_\Sigma \frac{x_j - y_j}{|x-y|^n} f(y) \, d\mathcal{H}^{n-1}(y) \quad \text{for } x \in \Sigma \setminus \operatorname{supp} f. \tag{1-6}$$

The above definition of the distributional Riesz transforms is very much in line with the point of view adopted in the statement of the classical $T(1)$ theorem of David and J.-L. Journé [1984]. Originally formulated in the entire Euclidean space, the latter result turned out to be remarkably resilient, in terms of the demands it places on the ambient space. Indeed, the $T(1)$ theorem has been subsequently generalized to spaces of homogeneous type (in the sense of Coifman and Weiss [1971; 1977]), a setting where only the existence of a quasidistance and a doubling measure is postulated (see, e.g., [Auscher and Hytönen 2013, Theorem 12.3; Christ 1990, Chapter IV; Han et al. 2008, Theorem 5.56, p. 166]). This is a framework in which an Ahlfors regular set $\Sigma \subset \mathbb{R}^n$, equipped with the Euclidean distance and the $(n-1)$-dimensional Hausdorff measure, fits in naturally.

As it turns out, much information (of both analytic and geometric flavor) is encapsulated in the action of the distributional Riesz transforms (1-4)–(1-5) on the constant function 1. Since the function 1 may not belong to $\mathscr{C}^\alpha_c(\Sigma)$ (which happens precisely when Σ is unbounded), one should be careful defining $R_j(1)$. In agreement with the procedures set in place by the $T(1)$ theorem, we consider $R_j(1)$ to be the linear functional acting on each function $g \in \mathscr{C}^\alpha_c(\Sigma)$ that satisfies the cancellation condition $\int_\Sigma g \, d\mathcal{H}^{n-1} = 0$

according to

$$\langle R_j(1), g\rangle := \frac{1}{2\omega_{n-1}}\int_\Sigma\int_\Sigma \frac{x_j-y_j}{|x-y|^n}[\phi(y)g(x)-\phi(x)g(y)]\,d\mathcal{H}^{n-1}(y)\,d\mathcal{H}^{n-1}(x) - \frac{1}{\omega_{n-1}}\int_\Sigma\int_\Sigma \frac{x_j-y_j}{|x-y|^n}(1-\phi(x))g(y)\,d\mathcal{H}^{n-1}(y)\,d\mathcal{H}^{n-1}(x), \tag{1-7}$$

where $\phi\in\mathscr{C}^\alpha_c(\Sigma)$ is an auxiliary function chosen to satisfy $\phi\equiv 1$ near $\operatorname{supp} g$. In this vein, let us remark that, in the case when Σ is compact, we do have $\mathscr{C}^\alpha_c(\Sigma)=\mathscr{C}^\alpha(\Sigma)$; hence, in particular, we now have $1\in\mathscr{C}^\alpha_c(\Sigma)$. In such a scenario, it may be readily verified that $R_j(1)$, defined as in (1-7), is the restriction of the functional $R_j1\in(\mathscr{C}^\alpha_c(\Sigma))^*$, defined as in (1-5) with $f=1$, to the space consisting of functions in $\mathscr{C}^\alpha_c(\Sigma)$ which integrate to zero. It is therefore reassuring to know that the various points of view on the nature of the action of the distributional Riesz transform R_j on the constant function 1 are consistent.

At the analytical level, the $T(1)$ theorem (for operators associated with odd kernels) gives that, for each fixed $j\in\{1,\dots,n\}$:

The distributional Riesz transform R_j from (1-4)–(1-5) extends to a bounded linear operator on $L^2(\Sigma)$ if and only if $R_j(1)\in\mathrm{BMO}(\Sigma)$, (1-8)

where $\mathrm{BMO}(\Sigma)$ is the John–Nirenberg space of functions of bounded mean oscillations on Σ (regarded as a space of homogeneous type).

At this stage, a few comments are in order, about the specific manner in which the various brands of Riesz transforms introduced earlier relate to one another. Assume that Σ is an Ahlfors regular subset of $\mathbb{R}^n$ which is countably rectifiable (of dimension $n-1$). First, it turns out that if for some $j\in\{1,\dots,n\}$ one (hence both) of the two equivalent conditions in (1-8) holds then the extension of the distributional Riesz transform R_j to a bounded linear operator on $L^2(\Sigma)$ (mentioned in (1-8)) is realized precisely by the principal value Riesz transform R^{pv}_j (defined for each $f\in L^2(\Sigma)$ as in (1-1) at $\mathcal{H}^{n-1}$-a.e. $x\in\Sigma$). In particular, for each $j\in\{1,\dots,n\}$:

If $\Sigma\subset\mathbb{R}^n$ is a compact Ahlfors regular set which is countably rectifiable (of dimension $n-1$) and $R_j(1)\in\mathrm{BMO}(\Sigma)$ then, for $\mathcal{H}^{n-1}$-a.e. $x\in\Sigma$,

$$R_j(1)(x)=\lim_{\varepsilon\to0^+}\int_{\substack{y\in\Sigma\\|y-x|>\varepsilon}}\frac{x_j-y_j}{|x-y|^n}\,d\mathcal{H}^{n-1}(y). \tag{1-9}$$

Second, if for some $j\in\{1,\dots,n\}$ the principal value Riesz transform R^{pv}_j, originally acting on $\mathscr{C}^\alpha_c(\Sigma)$, is known to extend to a bounded linear operator on $L^2(\Sigma)$, then R^{pv}_j coincides on $\mathscr{C}^\alpha_c(\Sigma)$ with the distributional Riesz transform R_j defined as in (1-4)–(1-5). Third, having fixed $j\in\{1,\dots,n\}$, the principal value Riesz transform R^{pv}_j extends to a bounded linear operator on $L^2(\Sigma)$ if and only if for each $\varepsilon>0$ the j-th truncated Riesz transform $R_{j,\varepsilon}$, defined as in (1-2), is bounded on $L^2(\Sigma)$ uniformly in ε, which happens if and only if the j-th maximal Riesz transform $R_{j,*}$ is bounded on $L^2(\Sigma)$, where, for each $f\in L^2(\Sigma)$,

$$R_{j,*}f(x):=\sup_{\varepsilon>0}|(R_{j,\varepsilon}f)(x)|,\quad x\in\Sigma. \tag{1-10}$$

All these results may be established via arguments of Calderón–Zygmund theory flavor, such as Cotlar's inequality, the Calderón–Zygmund decomposition, Marcinkiewicz's interpolation theorem and the boundedness of the Hardy–Littlewood maximal operator.

At the geometric level, the recent main result in [Nazarov et al. 2014] mentioned earlier may be rephrased, in light of (1-8), as follows: under the background assumption that Σ is an Ahlfors regular subset of $\mathbb{R}^n$, one has

$$\Sigma \text{ is a uniformly rectifiable set} \iff R_j(1) \in \mathrm{BMO}(\Sigma) \text{ for each } j \in \{1, \dots, n\}. \tag{1-11}$$

Hence, within the class of Ahlfors regular subsets of $\mathbb{R}^n$, the membership of all $R_j(1)$ to the John–Nirenberg space BMO characterizes uniform rectifiability. As mentioned previously in the introduction, this result refines earlier work of David and Semmes [1991], who proved that uniform rectifiability within the class of Ahlfors regular subsets of $\mathbb{R}^n$ is equivalent to the L^2-boundedness in that ambient of all truncated singular integral operators, uniform with respect to the truncation, (or, equivalently, the L^2-boundedness of all maximal operators), associated with all kernels of the form $k(x-y)$, where the function $k \in \mathscr{C}^\infty(\mathbb{R}^n \setminus \{0\})$ is odd and satisfies

$$\sup_{x\in\mathbb{R}^n\setminus\{0\}} \big[|x|^{(n-1)+|\gamma|}|(\partial^\gamma k)(x)|\big] < +\infty \quad \text{for all } \gamma \in \mathbb{N}_0^n. \tag{1-12}$$

In relation to the brands of Riesz transforms introduced earlier, the results of [David and Semmes 1991] imply[1] that, for each $j \in \{1, \dots, n\}$:

> Whenever Σ is a uniformly rectifiable set in $\mathbb{R}^n$, the principal value Riesz transform R_j^{pv} is a well-defined, linear and bounded operator on $L^2(\Sigma)$, which agrees on $\mathscr{C}_c^\alpha(\Sigma)$ with the distributional Riesz transform R_j. (1-13)

From the perspective of (1-11), one of the issues addressed by our first main result is that of extracting more geometric regularity for Σ if more analytic regularity for the $R_j(1)$ is available. We shall study this issue in the case when $\Sigma := \partial\Omega$, the topological boundary of an open subset Ω of $\mathbb{R}^n$. This fits into the paradigm of describing geometric characteristics (such as regularity of a certain nature) of a given set in terms of properties of suitable analytical entities (such as singular integral operators) associated with this environment. Specifically, we have the following theorem (for all relevant definitions the reader is referred to Section 2).

Theorem 1.1. *Assume $\Omega \subseteq \mathbb{R}^n$ is an Ahlfors regular domain with a compact boundary, satisfying $\partial\Omega = \partial(\overline{\Omega})$. Set $\sigma := \mathcal{H}^{n-1}\lfloor\partial\Omega$ and define $\Omega_+ := \Omega$ and $\Omega_- := \mathbb{R}^n \setminus \overline{\Omega}$.*

Then for each $\alpha \in (0, 1)$ the following claims are equivalent:

(a) *Ω is a domain of class $\mathscr{C}^{1+\alpha}$ (or a Lyapunov domain of order α).*

(b) *The distributional Riesz transforms, defined as in* (1-4)–(1-5) *with $\Sigma := \partial\Omega$, satisfy*

$$R_j 1 \in \mathscr{C}^\alpha(\partial\Omega) \quad \textit{for each } j \in \{1, \dots, n\}. \tag{1-14}$$

[1] In concert with the Calderón–Zygmund machinery alluded to earlier, and bearing in mind (2-48).

(c) Ω *is a* UR *domain and*, *given any odd homogeneous polynomial* P *of degree* $l \geq 1$ *in* $\mathbb{R}^n$, *the singular integral operator*

$$Tf(x) := \lim_{\varepsilon \to 0^+} \int_{\substack{y \in \partial\Omega \\ |x-y|>\varepsilon}} \frac{P(x-y)}{|x-y|^{n-1+l}} f(y)\, d\sigma(y), \quad x \in \partial\Omega, \tag{1-15}$$

is meaningfully defined for every $f \in \mathscr{C}^\alpha(\partial\Omega)$, *and maps* $\mathscr{C}^\alpha(\partial\Omega)$ *boundedly into itself.*

(d) Ω *is a* UR *domain and one has*

$$\mathscr{R}_j^{\pm} 1 \in \mathscr{C}^\alpha(\Omega_\pm) \quad \textit{for each } j \in \{1, \dots, n\}, \tag{1-16}$$

where, *for* $j \in \{1, \dots, n\}$,

$$\mathscr{R}_j^{\pm} f(x) := \frac{1}{\omega_{n-1}} \int_{\partial\Omega} \frac{x_j - y_j}{|x-y|^n} f(y)\, d\sigma(y), \quad x \in \Omega_\pm. \tag{1-17}$$

(e) Ω *is a* UR *domain and*, *for each odd homogeneous polynomial* P *of degree* $l \geq 1$ *in* $\mathbb{R}^n$, *the integral operators*

$$\mathbb{T}_\pm f(x) := \int_{\partial\Omega} \frac{P(x-y)}{|x-y|^{n-1+l}} f(y)\, d\sigma(y), \quad x \in \Omega_\pm, \tag{1-18}$$

map $\mathscr{C}^\alpha(\partial\Omega)$ *boundedly into* $\mathscr{C}^\alpha(\Omega_\pm)$.

Moreover, *if* Ω *is a* $\mathscr{C}^{1+\alpha}$ *domain for some* $\alpha \in (0, 1)$, *there exists a finite constant* $C > 0$, *depending only on* n, α, $\operatorname{diam}(\partial\Omega)$, *the upper Ahlfors regularity constant of* $\partial\Omega$, *and* $\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)}$ (*where* ν *is the outward unit normal to* Ω), *with the property that for each odd homogeneous polynomial* P *of degree* $l \geq 1$ *in* $\mathbb{R}^n$ *the integral operators* (1-18) *and* (1-15) *satisfy*

$$\|\mathbb{T}_\pm f\|_{\mathscr{C}^\alpha(\bar{\Omega}_\pm)} \leq C^l 2^{l^2} \|P\|_{L^2(S^{n-1})} \|f\|_{\mathscr{C}^\alpha(\partial\Omega)} \quad \textit{for all } f \in \mathscr{C}^\alpha(\partial\Omega), \tag{1-19}$$

$$\|Tf\|_{\mathscr{C}^\alpha(\partial\Omega)} \leq C^l 2^{l^2} \|P\|_{L^2(S^{n-1})} \|f\|_{\mathscr{C}^\alpha(\partial\Omega)} \quad \textit{for all } f \in \mathscr{C}^\alpha(\partial\Omega). \tag{1-20}$$

The operators described in (1-15) may be thought of as generalized Riesz transforms since they correspond to (1-15) with

$$P(x) := \frac{x_j}{\omega_{n-1}} \quad \text{for } x = (x_1, \dots, x_n) \in \mathbb{R}^n, \ 1 \leq j \leq n. \tag{1-21}$$

For the same choices of the polynomials, the claim in Theorem 1.1(e) implies that the harmonic single-layer operator (see (5-66) for a definition) is well-defined, linear and bounded as a mapping

$$\mathscr{S} : \mathscr{C}^\alpha(\partial\Omega) \longrightarrow \mathscr{C}^{1+\alpha}(\Omega_\pm). \tag{1-22}$$

In concert with the above comments, intended to clarify how the distributional Riesz transforms relate to the principal value Riesz transforms, Theorem 1.1 readily implies the following corollary:

Corollary 1.2. *Let* Ω *be a nonempty*, *proper*, *open subset of* $\mathbb{R}^n$ *with compact boundary*, *satisfying* $\partial\Omega = \partial(\overline{\Omega})$. *Then for every* $\alpha \in (0, 1)$ *the following statements are equivalent*:

(i) Ω *is a domain of class* $\mathscr{C}^{1+\alpha}$.

(ii) *Ω is an Ahlfors regular domain and, for each $j \in \{1, \dots, n\}$, the distributional Riesz transform R_j defined as in* (1-4)–(1-5) *with $\Sigma := \partial\Omega$ induces a linear and bounded operator in the context*

$$R_j : \mathscr{C}^\alpha(\partial\Omega) \longrightarrow \mathscr{C}^\alpha(\partial\Omega). \tag{1-23}$$

(iii) *Ω is an Ahlfors regular domain and*

$$R_j 1 \in \mathscr{C}^\alpha(\partial\Omega) \quad \textit{for each } j \in \{1, \dots, n\}. \tag{1-24}$$

(iv) *Ω is a* UR *domain and, for each $j \in \{1, \dots, n\}$, the principal value Riesz transform R_j^{pv} defined as in* (1-1) *with $\Sigma := \partial\Omega$ induces a linear and bounded operator in the context*

$$R_j^{\mathrm{pv}} : \mathscr{C}^\alpha(\partial\Omega) \longrightarrow \mathscr{C}^\alpha(\partial\Omega). \tag{1-25}$$

(v) *Ω is a* UR *domain and*

$$R_j^{\mathrm{pv}} 1 \in \mathscr{C}^\alpha(\partial\Omega) \quad \textit{for each } j \in \{1, \dots, n\}. \tag{1-26}$$

In dimension two, there is a variant of Theorem 1.1 starting from the demand that the boundary of the domain in question be an upper Ahlfors regular Jordan curve and, in lieu of the Riesz transforms, using the following version of the classical Cauchy integral operator in the principal value sense:

$$\mathfrak{C}^{\mathrm{pv}} f(z) := \lim_{\varepsilon\to 0^+} \frac{1}{2\pi i} \int_{\substack{\zeta\in\partial\Omega \\ |z-\zeta|>\varepsilon}} \frac{f(\zeta)}{\zeta - z}\, d\mathcal{H}^1(\zeta), \quad z \in \partial\Omega. \tag{1-27}$$

Theorem 1.3. *Let $\Omega \subseteq \mathbb{C}$ be a bounded open set whose boundary is an upper Ahlfors regular Jordan curve and fix $\alpha \in (0, 1)$. Then Ω is a domain of class $\mathscr{C}^{1+\alpha}$ if and only if the operator* (1-27) *satisfies $\mathfrak{C}^{\mathrm{pv}} 1 \in \mathscr{C}^\alpha(\partial\Omega)$.*

Under the initial background hypotheses on Ω made in Theorem 1.1, Ω being a $\mathscr{C}^1$ domain is equivalent to $\nu \in \mathscr{C}^0(\partial\Omega)$ (see [Hofmann et al. 2007] in this regard). This being said, the limiting case $\alpha = 0$ of the equivalence (a) $\Longleftrightarrow$ (b) in Theorem 1.1 requires replacing the space of continuous functions by the (larger) Sarason space VMO, of functions of vanishing mean oscillations (on $\partial\Omega$, viewed as a space of homogeneous type, in the sense of Coifman and Weiss, when equipped with the measure σ and the Euclidean distance). Specifically, the following result holds:

Theorem 1.4. *Let $\Omega \subseteq \mathbb{R}^n$ be an Ahlfors regular domain with a compact boundary, and denote by ν the geometric measure-theoretic outward unit normal to Ω. Then*

$$\nu \in \mathrm{VMO}(\partial\Omega) \textit{ and } \partial\Omega \textit{ is uniformly rectifiable} \iff R_j 1 \in \mathrm{VMO}(\partial\Omega) \textit{ for all } j \in \{1, \dots, n\}. \tag{1-28}$$

The equivalence (1-28) should be contrasted with (1-11). In the present context, the additional background assumption $\mathcal{H}^{n-1}(\partial\Omega \setminus \partial_*\Omega) = 0$ (which is part of the definition of an Ahlfors regular domain; see Definition 2.3) merely ensures that the geometric measure-theoretic outward unit normal ν to Ω is well-defined σ-a.e. on $\partial\Omega$.

The collection of all geometric conditions in Theorem 1.4, i.e., that $\Omega \subseteq \mathbb{R}^n$ is an Ahlfors regular domain such that $\partial\Omega$ is a uniformly rectifiable set, amounts to saying that Ω is a UR domain (see Definition 2.7).

Concerning this class of domains, it has been noted in [Hofmann et al. 2010, Corollary 3.9, p. 2633] that:

$$\text{If } \Omega \subset \mathbb{R}^n \text{ is an open set satisfying a two-sided corkscrew condition (in the sense of [Jerison and Kenig 1982]) and whose boundary is Ahlfors regular, then } \Omega \text{ is a UR domain.} \tag{1-29}$$

In fact, the same circle of techniques yielding Theorem 1.4 also allows us to characterize the class of regular SKT domains, originally introduced in [Hofmann et al. 2010, Definition 4.8, p. 2690] by demanding δ-Reifenberg flatness for some sufficiently small $\delta > 0$ (see Definition 7.6), Ahlfors regular boundary, and vanishing mean oscillations for the geometric measure-theoretic outward unit normal. Specifically, combining (1-29), Theorem 1.4, Theorem 7.7, and [Hofmann et al. 2010, Theorem 4.21, p. 2711] gives the following theorem:

Theorem 1.5. *If $\Omega \subseteq \mathbb{R}^n$ is an open set with a compact Ahlfors regular boundary, satisfying a two-sided John condition as described in Definition 7.3 (which, in particular, implies the two-sided corkscrew condition) then*

$$R_j 1 \in \mathrm{VMO}(\partial\Omega) \text{ for every } j \in \{1, \dots, n\} \iff \Omega \text{ is a regular SKT domain.} \tag{1-30}$$

It turns out that the equivalence (a) $\iff$ (b) in Theorem 1.1 essentially self-extends to the larger scale of Besov spaces $B_s^{p,p}(\partial\Omega)$ with $p \in [1, \infty]$ and $s \in (0, 1)$ satisfying $sp > n-1$, for which the Hölder spaces occur as a special, limiting case, corresponding to $p = \infty$. For a precise statement, see Theorem 7.11.

The category of singular integral operators falling under the scope of Theorem 1.1 already includes boundary layer potentials associated with basic PDEs of mathematical physics, such as the Laplacian, the Helmholtz operator, the Lamé system, the Stokes system, and even higher-order elliptic systems (see, e.g., [Colton and Kress 1983; Hsiao and Wendland 2008; Mitrea 2013; Mitrea and Mitrea 2013]). This being said, granted the estimates established in the last part of Theorem 1.1, the method of spherical harmonics then allows us to prove the following result, dealing with a more general class of operators:

Theorem 1.6. *Let Ω be a $\mathscr{C}^{1+\alpha}$ domain, $\alpha \in (0, 1)$, with compact boundary, and let $k \in \mathscr{C}^\infty(\mathbb{R}^n \setminus \{0\})$ be an odd function satisfying $k(\lambda x) = \lambda^{1-n} k(x)$ for all $\lambda \in (0, \infty)$ and $x \in \mathbb{R}^n \setminus \{0\}$. In addition, assume that there exists a sequence $\{m_l\}_{l \in \mathbb{N}_0} \subseteq \mathbb{N}_0$ for which*

$$\sum_{l=0}^{\infty} 4^{l^2} l^{-2m_l} \|(\Delta_{S^{n-1}})^{m_l}(k|_{S^{n-1}})\|_{L^2(S^{n-1})} < +\infty, \tag{1-31}$$

where $\Delta_{S^{n-1}}$ is the Laplace–Beltrami operator on the unit sphere S^{n-1} in $\mathbb{R}^n$.

Then the singular integral operators

$$\mathbb{T}f(x) := \int_{\partial\Omega} k(x-y) f(y)\, d\sigma(y), \qquad x \in \Omega, \tag{1-32}$$

$$Tf(x) := \lim_{\varepsilon \to 0^+} \int_{\substack{y \in \partial\Omega \\ |x-y| > \varepsilon}} k(x-y) f(y)\, d\sigma(y), \quad x \in \partial\Omega, \tag{1-33}$$

induce linear and bounded mappings

$$\mathbb{T} : \mathscr{C}^\alpha(\partial\Omega) \longrightarrow \mathscr{C}^\alpha(\overline{\Omega}) \quad \text{and} \quad T : \mathscr{C}^\alpha(\partial\Omega) \longrightarrow \mathscr{C}^\alpha(\partial\Omega). \tag{1-34}$$

We wish to note that Theorem 1.6 refines the implication (a) $\Longrightarrow$ (e) in Theorem 1.1 since, as explained in Remark 6.1, condition (1-31) is satisfied whenever the kernel k is of the form $P(x)/|x|^{n-1+l}$ for some homogeneous polynomial P of degree $l \in 2\mathbb{N}-1$ in $\mathbb{R}^n$. In fact, condition (1-31) holds for kernels k that are real-analytic away from 0 with lacunary Taylor series (involving sufficiently large gaps between the nonzero coefficients of their expansions, depending on n, α, $\operatorname{diam}(\partial\Omega)$, $\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)}$, and the upper Ahlfors regularity constant of $\partial\Omega$). Thus, the conclusions in Theorem 1.6 are valid for such kernels which are also odd and positive homogeneous of degree $1-n$.

Even though the statement does not reflect it, the proof of Theorem 1.1 makes essential use of the Clifford algebra $\mathcal{C}\ell_n$, a highly noncommutative generalization of the field of complex numbers to n dimensions, which also turns out to be geometrically sensitive. Indeed, this is a tool which has occasionally emerged at the core of a variety of problems at the interface between geometry and analysis. For us, one key aspect of this algebraic setting is the close relationship between the Riesz transforms and the principal value[2] Cauchy–Clifford integral operator $\mathcal{C}^{\mathrm{pv}}$ (defined in (5-2)). For the purpose of this introduction we single out the remarkable formula

$$\nu = -4\mathcal{C}^{\mathrm{pv}}\biggl(\sum_{j=1}^{n}(R_j^{pv}1)e_j\biggr) \quad \text{at } \sigma\text{-a.e. point on } \partial\Omega, \tag{1-35}$$

expressing the (geometric measure-theoretic) outward unit normal to Ω as the Clifford algebra cocktail $\sum_{j=1}^{n}(R_j^{\mathrm{pv}}1)e_j$ of principal value Riesz transforms acting on the constant function 1, coupled with the imaginary units e_j in $\mathcal{C}\ell_n$, then finally distorted through the action of the Cauchy–Clifford operator $\mathcal{C}^{\mathrm{pv}}$. Identity (1-35) plays a basic role in the proof of (b) $\Longrightarrow$ (a) in Theorem 1.1, together with a higher-dimensional generalization in a rough setting of the classical Plemelj–Privalov theorem stating that the principal value Cauchy integral operator on a piecewise smooth Jordan curve without cusps in the plane is bounded on Hölder spaces (see [Plemelj 1908; Privalov 1918; 1941]; see also [Iftimie 1965] for a higher-dimensional version for Lyapunov domains with compact boundaries). Specifically, in Theorem 5.6 we show that, whenever $\Omega \subset \mathbb{R}^n$ is a Lebesgue measurable set whose boundary is compact, upper Ahlfors regular, and satisfies $\mathcal{H}^{n-1}(\partial\Omega \setminus \partial_*\Omega) = 0$, it follows that for each $\alpha \in (0, 1)$ the principal value Cauchy–Clifford operator $\mathcal{C}^{\mathrm{pv}}$ induces a well-defined, linear and bounded mapping

$$\mathcal{C}^{\mathrm{pv}} : \mathscr{C}^\alpha(\partial\Omega) \otimes \mathcal{C}\ell_n \longrightarrow \mathscr{C}^\alpha(\partial\Omega) \otimes \mathcal{C}\ell_n. \tag{1-36}$$

The strategy employed in the proof of the implication (a) $\Longrightarrow$ (e) in Theorem 1.1 is somewhat akin to that of establishing a "$T(1)$-theorem" in the sense that matters are reduced to checking that $\mathbb{T}_\pm$ act reasonably on the constant function 1 (see (3-42) in this regard). In turn, this is accomplished via a proof by induction on $l \in 2\mathbb{N}-1$, the degree of the homogeneous polynomial P. The base case $l = 1$, corresponding to linear combinations of polynomials as in (1-21), is dealt with by viewing $(x_j - y_j)/|x-y|^n$ as a dimensional multiple of $\partial_j E_\Delta(x-y)$, where E_Δ is the standard fundamental solution for the Laplacian in $\mathbb{R}^n$. As such, the key cancellation property that eventually allows us to establish the desired Hölder estimate in this base case may be ultimately traced back to the PDE satisfied by $(x_j-y_j)/|x-y|^n$. In carrying out the inductive step

[2] In the standard sense of removing balls centered at the singularity and taking the limit as the radii shrink to zero.

we make essential use of elements of Clifford analysis permitting us to relate $\mathbb{T}_{\pm}1$ to the action of certain integral operators constructed as in (1-18) but relative to lower-degree polynomials acting on components of the outward unit normal ν to Ω. In this scenario, what allows the use of the induction hypothesis is the fact that, since Ω is a domain of class $\mathscr{C}^{1+\alpha}$, the components of the outward unit normal belong to $\mathscr{C}^{\alpha}(\partial\Omega)$.

The layout of the paper is as follows. Section 2 contains a discussion of background material of geometric measure-theoretic nature, along with some auxiliary lemmas which are relevant in our future endeavors. In Section 3 we first recall a version of the Calderón–Zygmund theory for singular integral operators on Lebesgue spaces in UR domains, and then proceed to establish several useful preliminary estimates for general singular integral operators. Next, Section 4 is reserved for a presentation of those aspects of Clifford analysis which are relevant for the present work. Section 5 is devoted to a study of Cauchy–Clifford integral operators (of both boundary-to-domain and boundary-to-boundary type) in the context of Hölder spaces. In contrast with the Calderón–Zygmund theory for singular integrals in UR domains reviewed in the first part of Section 3, the novelty here is the consideration of a much larger category of domains (see Theorem 5.6 for details). In the last part of Section 5 we also discuss the harmonic single and double layer potentials (involved in the initial induction step in the proof of the implication (a) $\Longrightarrow$ (e) in Theorem 1.1). Finally, in Section 6, the proofs of Theorems 1.1, 1.3 and 1.6 are presented, while Section 7 contains the proofs of Theorem 1.4 and the Besov space version of the equivalence (a) $\Longleftrightarrow$ (b) in Theorem 1.1 (see Theorem 7.11), and also a more general version of (1-30) in Theorem 7.7.

2. Geometric measure-theoretic preliminaries

Throughout, $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$ and we shall denote by $\mathbf{1}_E$ the characteristic function of a set E. For $\alpha \in (0,1)$ and $U \subseteq \mathbb{R}^n$ an arbitrary set (implicitly assumed to have cardinality at least 2), define the *homogeneous Hölder space of order* α on U as

$$\dot{\mathscr{C}}^{\alpha}(U) := \{u : U \to \mathbb{C} : [u]_{\dot{\mathscr{C}}^{\alpha}(U)} < +\infty\}, \tag{2-1}$$

where $[\,\cdot\,]_{\dot{\mathscr{C}}^{\alpha}(U)}$ stands for the seminorm

$$[u]_{\dot{\mathscr{C}}^{\alpha}(U)} := \sup_{\substack{x,y\in U\\ x\neq y}} \frac{|u(x)-u(y)|}{|x-y|^{\alpha}}. \tag{2-2}$$

The *inhomogeneous Hölder space of order* α on U is then defined as

$$\mathscr{C}^{\alpha}(U) := \{u \in \dot{\mathscr{C}}^{\alpha}(U) : u \text{ is bounded in } U\}, \tag{2-3}$$

and is equipped with the norm

$$\|u\|_{\mathscr{C}^{\alpha}(U)} := \sup_{U} |u| + [u]_{\dot{\mathscr{C}}^{\alpha}(U)} \quad \text{for all } u \in \mathscr{C}^{\alpha}(U). \tag{2-4}$$

Also, denote by $\mathscr{C}^{\alpha}_{c}(U)$ the subspace of $\mathscr{C}^{\alpha}(U)$ consisting of functions vanishing outside of a relatively compact subset of U. Moreover, if $\mathcal{O}$ is an open, nonempty subset of $\mathbb{R}^n$, then for given $\alpha \in (0,1)$ define

$$\mathscr{C}^{1+\alpha}(\mathcal{O}) := \{u \in \mathscr{C}^{1}(\mathcal{O}) : \|u\|_{\mathscr{C}^{1+\alpha}(\mathcal{O})} < +\infty\}, \tag{2-5}$$

where

$$\|u\|_{\mathscr{C}^{1+\alpha}(\mathcal{O})} := \sup_{x\in\mathcal{O}} |u(x)| + \sup_{x\in\mathcal{O}} |(\nabla u)(x)| + \sup_{\substack{x,y\in\mathcal{O}\\ x\neq y}} \frac{|(\nabla u)(x)-(\nabla u)(y)|}{|x-y|^{\alpha}}. \tag{2-6}$$

The following observations will be tacitly used in the sequel. For each set $U \subseteq \mathbb{R}^n$ and any $\alpha \in (0,1)$, we have that $\mathscr{C}^{\alpha}(U)$ is an algebra and the spaces $\dot{\mathscr{C}}^{\alpha}(U)$ and $\mathscr{C}^{\alpha}(U)$ are contained in the space of uniformly continuous functions on U, with $\dot{\mathscr{C}}^{\alpha}(U) = \dot{\mathscr{C}}^{\alpha}(\overline{U})$ and $\mathscr{C}^{\alpha}(U) = \mathscr{C}^{\alpha}(\overline{U})$. Moreover, $\dot{\mathscr{C}}^{\alpha}(U) = \mathscr{C}^{\alpha}(U)$ if U is bounded. Finally, we shall make no notational distinction between a Hölder space of scalar functions and its version involving vector-valued functions. A similar convention is employed for other function spaces used in this work.

Definition 2.1. A nonempty, open, proper subset Ω of $\mathbb{R}^n$ is called a *domain of class* $\mathscr{C}^{1+\alpha}$ for some $\alpha \in (0,1)$ (or a *Lyapunov domain of order* α), if there exist $r, h > 0$ with the following significance. For every point $x_0 \in \partial\Omega$ one can find a coordinate system $(x_1,\dots,x_n) = (x', x_n)$ in $\mathbb{R}^n$ which is isometric to the canonical one and has origin at x_0, along with a real-valued function $\varphi \in \mathscr{C}^{1+\alpha}(\mathbb{R}^{n-1})$ such that

$$\Omega \cap \mathcal{C}(r,h) = \{x = (x', x_n) \in \mathbb{R}^{n-1}\times\mathbb{R} : |x'| < r \text{ and } \varphi(x') < x_n < h\}, \tag{2-7}$$

where $\mathcal{C}(r,h)$ stands for the cylinder

$$\{x = (x', x_n) \in \mathbb{R}^{n-1}\times\mathbb{R} : |x'| < r \text{ and } -h < x_n < h\}. \tag{2-8}$$

Strictly speaking, the traditional definition of a Lyapunov[3] domain $\Omega \subseteq \mathbb{R}^n$ of order α requires that $\partial\Omega$ is locally given by the graph of a differentiable function $\varphi : \mathbb{R}^{n-1} \to \mathbb{R}$ whose normal ν to its graph Σ has the property that the acute angle $\theta_{x,y}$ between $\nu(x)$ and $\nu(y)$ for two arbitrary points $x, y \in \Sigma$ satisfies $\theta_{x,y} \le C|x-y|^{\alpha}$; see, e.g., [Iftimie 1965, Définition 2.1, p. 301]. This being said, it is easy to see that the latter condition implies that ν is Hölder continuous of order α and, ultimately, that Ω is a domain of class $\mathscr{C}^{1+\alpha}$ in the sense of our Definition 2.1.

We shall now present a brief summary of a number of definitions and results from geometric measure theory which are relevant for the current work (see the monographs of H. Federer [1969], W. Ziemer [1989], L. Evans and R. Gariepy [1992] for more details). We say a Lebesgue measurable set $\Omega \subset \mathbb{R}^n$ has *locally finite perimeter* provided $\nabla\mathbf{1}_{\Omega}$ is a locally finite, Borel regular, $\mathbb{R}^n$-valued measure. Given a Lebesgue measurable set $\Omega \subset \mathbb{R}^n$ of locally finite perimeter we denote by σ the total variation measure of $\nabla\mathbf{1}_{\Omega}$. Then σ is a locally finite positive measure, supported on $\partial\Omega$. In the sequel, we shall frequently identify σ with its restriction to $\partial\Omega$, with no special mention. By $L^p(\partial\Omega,\sigma)$, where $0 < p \le \infty$, we shall denote the usual scale of Lebesgue spaces on $\partial\Omega$ with respect to the measure σ.

Clearly, each component of $\nabla\mathbf{1}_{\Omega}$ is absolutely continuous with respect to σ, so from the Radon–Nikodym theorem it follows that

$$\nabla\mathbf{1}_{\Omega} = -\nu\sigma, \tag{2-9}$$

[3] Also spelled as Liapunov.

where

$$\nu \text{ is an } \mathbb{R}^n\text{-valued function with components in } L^\infty(\partial\Omega,\sigma) \text{ and which satisfies } |\nu(x)|=1 \text{ at } \sigma\text{-a.e. point } x\in\partial\Omega. \tag{2-10}$$

Moreover, Besicovitch's differentiation theorem implies that at σ-a.e. point $x \in \partial\Omega$ we have

$$\lim_{r\to 0^+} ⨍_{B(x,r)} \nu(y)\,d\sigma(y) = \nu(x), \tag{2-11}$$

where the barred integral indicates mean average. We shall refer to ν and σ as the (geometric measure-theoretic) *outward unit normal* to Ω and the *surface measure* on $\partial\Omega$, respectively.

Next, denote by $\mathscr{L}^n$ the Lebesgue measure in $\mathbb{R}^n$ and recall that the *measure-theoretic boundary* $\partial_*\Omega$ of a Lebesgue measurable set $\Omega \subseteq \mathbb{R}^n$ is defined by

$$\partial_*\Omega := \left\{x\in\partial\Omega : \limsup_{r\to 0^+} \frac{\mathscr{L}^n(B(x,r)\cap\Omega)}{r^n} > 0 \text{ and } \limsup_{r\to 0^+} \frac{\mathscr{L}^n(B(x,r)\setminus\Omega)}{r^n} > 0\right\}. \tag{2-12}$$

Also, the *reduced boundary* $\partial^*\Omega$ of Ω is defined as

$$\partial^*\Omega := \{x\in\partial\Omega : \text{(2-11) holds and } |\nu(x)|=1\}. \tag{2-13}$$

As is well-known (see [Ziemer 1989, Lemma 5.9.5, p. 252; Evans and Gariepy 1992, p. 208]), one has

$$\partial^*\Omega \subseteq \partial_*\Omega \subseteq \partial\Omega \quad\text{and}\quad \mathcal{H}^{n-1}(\partial_*\Omega\setminus\partial^*\Omega)=0, \tag{2-14}$$

where $\mathcal{H}^{n-1}$ is the $(n-1)$-dimensional Hausdorff measure in $\mathbb{R}^n$. Also,

$$\sigma = \mathcal{H}^{n-1}\lfloor\partial^*\Omega. \tag{2-15}$$

Hence, if Ω has locally finite perimeter, it follows from (2-14) that the outward unit normal is defined σ-a.e. on $\partial_*\Omega$. In particular, if

$$\mathcal{H}^{n-1}(\partial\Omega\setminus\partial_*\Omega)=0, \tag{2-16}$$

then from (2-13)–(2-14) we see that the outward unit normal ν is defined σ-a.e. on $\partial\Omega$, and (2-15) becomes $\sigma = \mathcal{H}^{n-1}\lfloor\partial\Omega$. Works of Federer and De Giorgi also give that

$$\partial^*\Omega \text{ is } \textit{countably rectifiable} \text{ (of dimension } n-1), \tag{2-17}$$

in the sense that it is a countable disjoint union

$$\partial^*\Omega = N \cup \Bigl(\bigcup_{k\in\mathbb{N}} M_k\Bigr) \tag{2-18}$$

where each M_k is a compact subset of an $(n-1)$-dimensional $\mathscr{C}^1$ surface in $\mathbb{R}^n$ and $\mathcal{H}^{n-1}(N)=0$. It then happens that ν is normal to each such surface, in the usual sense. For further reference let us remark here that, as is apparent from (2-17), (2-14), and (2-18):

If $\Omega \subset \mathbb{R}^n$ is a Lebesgue measurable set which has locally finite perimeter and for which (2-16) holds, then $\partial\Omega$ is countably rectifiable (of dimension $n-1$). (2-19)

The following characterization of the class of $\mathscr{C}^{1+\alpha}$ domains from [Hofmann et al. 2007] is going to play an important role for us here.

Theorem 2.2. *Assume that Ω is a nonempty, open, proper subset of $\mathbb{R}^n$ of locally finite perimeter, with compact boundary, for which*

$$\partial\Omega = \partial(\bar{\Omega}), \tag{2-20}$$

and denote by ν the geometric measure-theoretic outward unit normal to $\partial\Omega$, as defined in (2-9)–(2-10). *Also, fix $\alpha \in (0, 1)$. Then Ω is a $\mathscr{C}^{1+\alpha}$ domain if and only if, after altering ν on a set of σ-measure zero, one has $\nu \in \mathscr{C}^{\alpha}(\partial\Omega)$.*

Condition (2-20) is designed to preclude pathological happenstances such as a slit disk. By the Jordan–Brouwer separation theorem (see [Alexander 1978, Theorem 1, p. 284]), (2-20) is automatically satisfied if $\partial\Omega$ is a compact, connected, $(n-1)$-dimensional topological manifold without boundary (since in this scenario $\mathbb{R}^n \setminus \partial\Omega$ consists of precisely two components, each with boundary $\partial\Omega$; see [Alvarado et al. 2011] for details).

Changing topics, we remind the reader that a set $\Sigma \subset \mathbb{R}^n$ is called *Ahlfors regular* provided it is closed, nonempty, and there exists $C \in (1, \infty)$ such that

$$C^{-1} r^{n-1} \le \mathcal{H}^{n-1}(B(x, r) \cap \Sigma) \le C\, r^{n-1} \tag{2-21}$$

for each $x \in \Sigma$ and $r \in (0, \operatorname{diam} \Sigma)$. When considered by itself, the second inequality above will be referred to as *upper Ahlfors regularity*. In this vein, we wish to remark that (see [Evans and Gariepy 1992, Theorem 1, p. 222]):

> Any Lebesgue measurable subset of $\mathbb{R}^n$ with an upper Ahlfors regular boundary is of locally finite perimeter. (2-22)

It is natural to make the following definition:

Definition 2.3. Call an open, nonempty, proper subset Ω of $\mathbb{R}^n$ an *Ahlfors regular domain* provided $\partial\Omega$ is an Ahlfors regular set and $\mathcal{H}^{n-1}(\partial\Omega \setminus \partial_*\Omega) = 0$.

Let us remark here that (2-19) and (2-22) imply the following result:

> If $\Omega \subset \mathbb{R}^n$ is a Lebesgue measurable set with an upper Ahlfors regular boundary satisfying $\mathcal{H}^{n-1}(\partial\Omega \setminus \partial_*\Omega) = 0$, then Ω is a set of locally finite perimeter and its topological boundary, $\partial\Omega$, is countably rectifiable (of dimension $n-1$). (2-23)

For further use, we record the following consequence of (2-23) and Definition 2.3:

> Any Ahlfors regular domain in $\mathbb{R}^n$ has a countably rectifiable topological boundary (of dimension $n-1$). (2-24)

Later on, the following result is going to be of significance to us:

Proposition 2.4. *Let $\Sigma \subseteq \mathbb{R}^n$ be an Ahlfors regular set which is countably rectifiable (of dimension $n-1$). Define $\sigma := \mathcal{H}^{n-1}\lfloor\Sigma$ and consider an arbitrary function $f \in L^1_{\mathrm{loc}}(\Sigma, \sigma)$. Then, for each $j \in \{1, \dots, n\}$,*

$$\lim_{\varepsilon\to 0^+}\Big\{\sup_{r\in(\varepsilon/2,\varepsilon)}\Big|\int_{\substack{y\in\Sigma\\ \varepsilon/4<|y-x|\le r}} \frac{x_j-y_j}{|x-y|^n} f(y)\,d\sigma(y)\Big|\Big\} = 0 \quad \textit{for } \sigma\textit{-a.e. } x \in \Sigma. \tag{2-25}$$

Proof. Fix $j \in \{1, \dots, n\}$ and pick some large $R > 0$. For each $\varepsilon \in (0, 1)$, $r \in \left(\frac{1}{2}\varepsilon, \varepsilon\right)$, and $x \in \Sigma \cap B(0, R)$ split

$$\int_{\substack{y\in\Sigma\\ \varepsilon/4<|y-x|\le r}} \frac{x_j-y_j}{|x-y|^n} f(y)\,d\sigma(y) = I_{\varepsilon,r} + II_{\varepsilon,r}, \tag{2-26}$$

where

$$I_{\varepsilon,r} := \int_{\substack{y\in\Sigma\\ \varepsilon/4<|y-x|\le r}} \frac{x_j-y_j}{|x-y|^n}(f(y)-f(x))\,d\sigma(y), \tag{2-27}$$

$$II_{\varepsilon,r} := f(x)\Big\{\int_{\substack{y\in\Sigma\cap B(0,R+1)\\ \varepsilon/4<|y-x|<1}} \frac{x_j-y_j}{|x-y|^n}\,d\sigma(y) - \int_{\substack{y\in\Sigma\cap B(0,R+1)\\ r<|y-x|<1}} \frac{x_j-y_j}{|x-y|^n}\,d\sigma(y)\Big\}. \tag{2-28}$$

The left-to-right implication in (1-3), used for the set $\Sigma\cap B(0, R+1)$, gives that σ-a.e. point $x \in \Sigma\cap B(0, R)$ has the property that, for each $\delta > 0$, there exists $\theta_\delta \in (0, 1)$ such that, for each $\theta_1, \theta_2 \in (0, \theta_\delta)$, we have

$$\Big|\int_{\substack{y\in\Sigma\cap B(0,R+1)\\ \theta_1<|y-x|<1}} \frac{x_j-y_j}{|x-y|^n}\,d\sigma(y) - \int_{\substack{y\in\Sigma\cap B(0,R+1)\\ \theta_2<|y-x|<1}} \frac{x_j-y_j}{|x-y|^n}\,d\sigma(y)\Big| < \delta. \tag{2-29}$$

In turn, this readily yields

$$\lim_{\varepsilon\to 0^+}\Big\{\sup_{r\in(\varepsilon/2,\varepsilon)} |II_{\varepsilon,r}|\Big\} = 0 \quad \text{for } \sigma\text{-a.e. } x \in \Sigma\cap B(0, R). \tag{2-30}$$

Next, thanks to the upper Ahlfors regularity condition satisfied by Σ, we may estimate (recall that the barred integral stands for mean average)

$$|I_{\varepsilon,r}| \le \left(\frac{4}{\varepsilon}\right)^{n-1}\int_{\Sigma\cap B(x,\varepsilon)} |f(y)-f(x)|\,d\sigma(y) \le c\,⨍_{\Sigma\cap B(x,\varepsilon)} |f(y)-f(x)|\,d\sigma(y). \tag{2-31}$$

Hence, on the one hand,

$$\lim_{\varepsilon\to 0^+}\Big\{\sup_{r\in(\varepsilon/2,\varepsilon)} |I_{\varepsilon,r}|\Big\} = 0 \quad \text{if } x \text{ is a Lebesgue point for } f. \tag{2-32}$$

On the other hand, the triplet $(\Sigma, |\cdot-\cdot|, \sigma)$ is a space of homogeneous type and the underlying measure is Borel regular. As such, Lebesgue's differentiation theorem gives that σ-a.e. point in Σ is a Lebesgue point for f. Bearing this in mind, the desired conclusion now follows from (2-26), (2-30), and (2-32). □

In the treatment of the principal value Cauchy–Clifford integral operator in Section 5, the following lemma plays a significant role:

Lemma 2.5. *Let $\Omega \subset \mathbb{R}^n$ be a Lebesgue measurable set of locally finite perimeter such that* (2-16) *holds. Then, for each $x \in \partial^*\Omega$, there exists a Lebesgue measurable set $\mathcal{O}_x \subset (0,1)$ of density* 1 *at* 0, *i.e., satisfying*

$$\lim_{\varepsilon\to 0^+} \frac{\mathscr{L}^1(\mathcal{O}_x \cap (0,\varepsilon))}{\varepsilon} = 1, \tag{2-33}$$

with the property that

$$\lim_{\substack{r\to 0^+\\ r\in\mathcal{O}_x}} \frac{\mathcal{H}^{n-1}(\Omega \cap \partial B(x,r))}{\omega_{n-1} r^{n-1}} = \frac{1}{2}. \tag{2-34}$$

Proof. We largely follow a suggestion of Taylor (personal communication, 2015). Given $x \in \partial^*\Omega$, there exists an approximate tangent plane π to Ω at x (see the discussion in [Hofmann et al. 2010, p. 2627]) and we denote by $\pi^\pm$ the two half-spaces into which π divides $\mathbb{R}^n$ (with the convention that the outward unit normal to π^- is $\nu(x)$). For each $r > 0$, set $\partial^\pm B(x,r) := \partial B(x,r) \cap \pi^\pm$ and introduce

$$W(x,r) := \partial^- B(x,r) \triangle (\Omega \cap \partial B(x,r)), \tag{2-35}$$

where, generally speaking, $U \triangle V$ denotes the symmetric difference $(U \setminus V) \cup (V \setminus U)$. With this notation, in the proof of [Hofmann et al. 2010, Proposition 3.3, p. 2628] it has been shown that

$$\int_0^R \mathcal{H}^{n-1}(W(x,r))\,dr = o(R^n) \quad \text{as } R \to 0^+. \tag{2-36}$$

Thus, if we consider the function

$$\phi : (0,1) \to [0,\infty), \qquad \phi(r) := r^{1-n}\mathcal{H}^{n-1}(W(x,r)) \quad \text{for each } r \in (0,1), \tag{2-37}$$

it follows from (2-36) that

$$\int_{R/2}^R \phi(r)\,dr \le \Big(\frac{R}{2}\Big)^{1-n} \int_0^R \mathcal{H}^{n-1}(W(x,r))\,dr = o(R) \quad \text{as } R \to 0^+. \tag{2-38}$$

We introduce the dyadic intervals $I_k := [2^{-(k+1)}, 2^{-k}]$ for $k \in \mathbb{N}_0$ and note that (2-38) entails

$$\delta_k := \fint_{I_k} \phi(r)\,dr \longrightarrow 0^+ \quad \text{as } k \to \infty. \tag{2-39}$$

For each $k \in \mathbb{N}_0$ split

$$I_k = A_k \cup B_k \qquad \text{with} \qquad B_k := \{r \in I_k : \phi(r) > \sqrt{\delta_k}\} \quad \text{and} \quad A_k := I_k \setminus B_k. \tag{2-40}$$

Then Chebyshev's inequality permits us to estimate

$$\frac{\mathscr{L}^1(B_k)}{\mathscr{L}^1(I_k)} \le \frac{1}{\sqrt{\delta_k}} \fint_{I_k} \phi(r)\,dr = \sqrt{\delta_k} \quad \text{for all } k \in \mathbb{N}_0. \tag{2-41}$$

In light of (2-39), this implies that if we now define

$$\mathcal{O}_x := \bigcup_{k\in\mathbb{N}_0} A_k \subset (0,1), \tag{2-42}$$

then

$$\lim_{\substack{r\to 0^+\\ r\in\mathcal{O}_x}} \phi(r)=0. \tag{2-43}$$

We claim that (2-33) also holds for this choice of $\mathcal{O}_x$. To see that this is the case, assume that some arbitrary $\theta>0$ has been fixed. For each $\varepsilon\in(0,1)$, let $N_\varepsilon\in\mathbb{N}_0$ be such that $2^{-N_\varepsilon-1}<\varepsilon\leq 2^{-N_\varepsilon}$. Since $N_\varepsilon\to\infty$ as $\varepsilon\to 0^+$, it follows from (2-39) that there exists $\varepsilon_\theta>0$ with the property that

$$\delta_k\leq\theta^2 \quad\text{whenever}\quad 0<\varepsilon<\varepsilon_\theta \ \text{ and } \ k\geq N_\varepsilon. \tag{2-44}$$

Assuming that $0<\varepsilon<\varepsilon_\theta$ we may then estimate

$$\begin{aligned} 0\leq\frac{\varepsilon-\mathscr{L}^1(\mathcal{O}_x\cap(0,\varepsilon))}{\varepsilon}&=\varepsilon^{-1}\mathscr{L}^1((0,\varepsilon)\setminus\mathcal{O}_x)\\ &\leq\varepsilon^{-1}\mathscr{L}^1((0,2^{-N_\varepsilon})\setminus\mathcal{O}_x)=\varepsilon^{-1}\sum_{k=N_\varepsilon}^{\infty}\mathscr{L}^1(B_k)\\ &\leq\varepsilon^{-1}\sum_{k=N_\varepsilon}^{\infty}\mathscr{L}^1(I_k)\sqrt{\delta_k}\leq\varepsilon^{-1}\theta 2^{-N_\varepsilon}\leq\frac{\theta}{2}. \end{aligned} \tag{2-45}$$

This finishes the proof of (2-33). At this stage, there remains to observe that since, generally speaking, $|\mathscr{H}^{n-1}(U)-\mathscr{H}^{n-1}(V)|\leq\mathscr{H}^{n-1}(U\Delta V)$, from (2-35) we have

$$\left|\frac{\mathcal{H}^{n-1}(\Omega\cap\partial B(x,r))}{\omega_{n-1}r^{n-1}}-\frac{1}{2}\right|\leq\frac{\mathcal{H}^{n-1}(W(x,r))}{\omega_{n-1}r^{n-1}}=\frac{1}{\omega_{n-1}}\phi(r) \tag{2-46}$$

for each $r\in(0,1)$. Then (2-34) is a consequence of this and (2-43). □

Following [David and Semmes 1991] we now make the following definition:

Definition 2.6. Call a subset Σ of $\mathbb{R}^n$ a *uniformly rectifiable set* provided it is Ahlfors regular and the following holds: there exist $\varepsilon, M\in(0,\infty)$ such that, for each $x\in\Sigma$ and $R\in(0,\operatorname{diam}\Sigma)$, there is a Lipschitz map $\varphi: B_R^{n-1}\to\mathbb{R}^n$ (where B_R^{n-1} is a ball of radius R in $\mathbb{R}^{n-1}$) with Lipschitz constant at most M, such that

$$\mathcal{H}^{n-1}\big(\Sigma\cap B(x,R)\cap\varphi(B_R^{n-1})\big)\geq\varepsilon R^{n-1}. \tag{2-47}$$

Informally speaking, uniform rectifiability is about the ability of identifying big pieces of Lipschitz images inside the given set (in a uniform, scale-invariant fashion) and can be thought of as a quantitative version of countable rectifiability. From [Hofmann et al. 2010, p. 2629] we know that:

Any uniformly rectifiable set $\Sigma\subset\mathbb{R}^n$ is countably rectifiable (of dimension $n-1$). (2-48)

Following [Hofmann et al. 2010], we shall also make the following definition:

Definition 2.7. We call a nonempty open proper subset Ω of $\mathbb{R}^n$ a UR (*uniformly rectifiable*) *domain* provided Ω is an Ahlfors regular domain whose topological boundary, $\partial\Omega$, is a uniformly rectifiable set.

For further use, it is useful to point out that, as is apparent from definitions:

If $\Omega \subset \mathbb{R}^n$ is a UR domain with $\partial\Omega = \partial(\overline{\Omega})$ then $\mathbb{R}^n \setminus \overline{\Omega}$ is a UR domain with the same boundary. (2-49)

We now turn to the notion of nontangential boundary trace of functions defined in a nonempty, proper, open set $\Omega \subset \mathbb{R}^n$. Fix $\kappa > 0$ and for each boundary point $x \in \partial\Omega$ introduce the nontangential approach region

$$\Gamma_\kappa(x) := \{y \in \Omega : |x - y| < (1+\kappa)\,\mathrm{dist}(y, \partial\Omega)\}. \tag{2-50}$$

It should be noted that, under the current hypotheses, it could happen that $\Gamma_\kappa(x) = \varnothing$ for points $x \in \partial\Omega$ (as is the case if, e.g., Ω has a suitable cusp with vertex at x). Next, given a Lebesgue measurable function $u : \Omega \to \mathbb{R}$, we wish to consider its limit at boundary points $x \in \partial\Omega$ taken from within nontangential approach regions with vertex at x. For such a limit to be meaningfully defined at σ-a.e. point on $\partial\Omega$ (where, as usual, $\sigma := \mathcal{H}^{n-1}\lfloor\partial\Omega$), it is necessary that

$$x \in \overline{\Gamma}_\kappa(x) \quad \text{for } \sigma\text{-a.e. } x \in \partial\Omega. \tag{2-51}$$

We shall call an open set $\Omega \subseteq \mathbb{R}^n$ satisfying (2-51) above *weakly accessible*. Assuming that this is the case, we say that u has a nontangential boundary trace almost everywhere on $\partial\Omega$ if for σ-a.e. point $x \in \partial\Omega$ there exists some $N(x) \subset \Gamma_\kappa(x)$ of measure zero such that the limit

$$\big(u\big|^{\mathrm{nt}}_{\partial\Omega}\big)(x) := \lim_{\substack{y\to x\\ y\in\Gamma_\kappa(x)\setminus N(x)}} u(y) \quad \text{exists.} \tag{2-52}$$

When u is a continuous function in Ω, we may take $N(x) = \varnothing$. For future use, let us also define the nontangential maximal operator of u as

$$(\mathcal{N}u)(x) := \|u\|_{L^\infty(\Gamma_\kappa(x))} \in [0, \infty] \quad \text{for all } x \in \partial\Omega, \tag{2-53}$$

where the essential supremum (taken to be 0 if $\Gamma_\kappa(x) = \varnothing$) in the right-hand side is taken with respect to the Lebesgue measure in $\mathbb{R}^n$.

The following result has been proved in [Hofmann et al. 2010, Proposition 2.9, p. 2588]:

Proposition 2.8. *Any Ahlfors regular domain is weakly accessible. As a corollary, any* UR *domain is weakly accessible.*

We continue by recording the definition of the class of uniform domains introduced by O. Martio and J. Sarvas [1979].

Definition 2.9. Call a nonempty, proper, open set $\Omega \subseteq \mathbb{R}^n$ a *uniform domain* if there exists a constant $c \in (0, \infty)$ with the property:

For each $x, y \in \Omega$ there exists a rectifiable curve $\gamma : [0, 1] \to \Omega$ joining x and y such that $\mathrm{length}(\gamma) \le c|x - y|$ and which has the property

$$\min\{\mathrm{length}(\gamma_{x,z}),\ \mathrm{length}(\gamma_{z,y})\} \le c\,\mathrm{dist}(z, \partial\Omega) \tag{2-54}$$

for all $z \in \gamma([0, 1])$, where $\gamma_{x,z}$ and $\gamma_{z,y}$ are the two components of the path $\gamma([0, 1])$ joining x with z, and z with y, respectively.

Condition (2-54) asserts that the length of $\gamma([0, 1])$ is comparable to the distance between its endpoints and that, away from its endpoints, the curve γ stays correspondingly far from $\partial\Omega$. Hence, heuristically, condition (2-54) implies that points in Ω can be joined in Ω by a curvilinear (or twisted) double cone which is neither too crocked nor too thin. Here we wish to note that, given an open nonempty subset Ω of $\mathbb{R}^n$ with compact boundary along with some $\alpha \in (0, 1)$, the following implication holds:

$$\Omega \text{ is a } \mathscr{C}^{1+\alpha} \text{ domain} \implies \Omega \text{ is a uniform domain.} \tag{2-55}$$

Throughout, we make the convention that, given a nonempty, proper subset Ω of $\mathbb{R}^n$, we abbreviate

$$\rho(z) := \mathrm{dist}(z, \partial\Omega) \quad \text{for every } z \in \Omega. \tag{2-56}$$

Lemma 2.10. *Let $\Omega \subset \mathbb{R}^n$ be a uniform domain. Then for each $\alpha \in (0, 1)$ there exists a finite constant $C > 0$, depending only on α and Ω, such that the estimate*

$$[u]_{\dot{\mathscr{C}}^\alpha(\Omega)} \le C \sup_{x\in\Omega}\{\rho(x)^{1-\alpha}|\nabla u(x)|\} \tag{2-57}$$

holds for every function $u \in \mathscr{C}^1(\Omega)$.

Proof. Consider $c > 0$ such that condition (2-54) is satisfied. Let $x, y \in \Omega$ be two arbitrary points and assume that γ is as in Definition 2.9. Denote by L and s the length of the curve $\gamma^* := \gamma([0, 1])$ and the arc-length parameter on γ^*, respectively, with $s \in [0, L]$. Also, let $s \mapsto \gamma(s) \in \gamma^*$ be the canonical arc-length parametrization of γ^*. In particular, $s \mapsto \gamma(s)$ is absolutely continuous, $|d\gamma/ds| = 1$ for almost every s and, for every continuous function f in Ω,

$$\int_{\gamma^*} f := \int_0^L f(\gamma(s))\,ds. \tag{2-58}$$

Thus, from (2-54) and (2-58), for each $\alpha \in (0, 1)$ we have

$$\begin{aligned}\int_{\gamma^*} \rho^{\alpha-1} &= \int_0^L \rho(\gamma(s))^{\alpha-1}\,ds \le c^{1-\alpha}\int_0^L (\min\{s, L-s\})^{\alpha-1}\,ds \\ &\le 2c^{1-\alpha}\int_0^{L/2} s^{\alpha-1}\,ds = C(c,\alpha)L^\alpha \le C(c,\alpha)|x-y|^\alpha. \end{aligned} \tag{2-59}$$

Then, since $|d\gamma/ds| = 1$ for almost every s, for every $u \in \mathscr{C}^1(\Omega)$ we may write

$$\begin{aligned} |u(x) - u(y)| = \left| \int_0^L \frac{d}{ds}[u(\gamma(s))]\,ds \right| \le \int_0^L |(\nabla u)(\gamma(s))|\,ds = \int_{\gamma^*} |\nabla u| \\ \le \sup_{\gamma^*}\{|\nabla u|\rho^{1-\alpha}\} \int_{\gamma^*} \rho^{\alpha-1} \\ \le C|x-y|^\alpha \big\| |\nabla u|\rho^{1-\alpha} \big\|_{L^\infty(\Omega)}, \end{aligned} \tag{2-60}$$

finishing the proof of (2-57). □

Recall that for each $k \in \mathbb{N}$ we let $\mathscr{L}^k$ stand for the k-dimensional Lebesgue measure in $\mathbb{R}^k$. Also, we shall let $\langle \cdot\,, \cdot \rangle$ denote the standard inner product of vectors in $\mathbb{R}^n$.

Lemma 2.11. *Assume that $D \subseteq \mathbb{R}^n$ is a set of locally finite perimeter. Denote by ν its geometric measure-theoretic outward unit normal and define $\sigma := \mathcal{H}^{n-1}\lfloor\partial_* D$. Also, suppose that $\vec{F} \in \mathscr{C}^1_0(\mathbb{R}^n, \mathbb{R}^n)$. Then, for each $x \in \mathbb{R}^n$,*

$$\int_{D\cap B(x,r)} \operatorname{div}\vec{F}\,d\mathscr{L}^n = \int_{\partial_* D\cap B(x,r)} \langle \vec{F}, \nu\rangle\,d\sigma + \int_{D\cap\partial B(x,r)} \langle \vec{F}, \nu\rangle\,d\mathcal{H}^{n-1} \tag{2-61}$$

and

$$\int_{D\setminus B(x,r)} \operatorname{div}\vec{F}\,d\mathscr{L}^n = \int_{\partial_* D\setminus B(x,r)} \langle \vec{F}, \nu\rangle\,d\sigma - \int_{D\cap\partial B(x,r)} \langle \vec{F}, \nu\rangle\,d\mathcal{H}^{n-1} \tag{2-62}$$

for $\mathscr{L}^1$-a.e. $r \in (0, \infty)$, where ν in each of the last integrals in the above right-hand sides is the outward unit normal to $B(x, r)$.

Proof. Identity (2-61) is simply [Evans and Gariepy 1992, Lemma 1, p. 195]. Then (2-62) follows by combining this with the Gauss–Green formula [Evans and Gariepy 1992, Theorem 1, p. 209]. □

We conclude this section by recording the following two-dimensional result, which is going to be relevant when dealing with the proof of Theorem 1.3.

Proposition 2.12. *Let $\Omega \subseteq \mathbb{C}$ be a bounded open set whose boundary is an upper Ahlfors regular Jordan curve. Then Ω is a simply connected* UR *domain satisfying $\partial\Omega = \partial(\overline{\Omega})$. Hence, in particular, $\mathcal{H}^1(\partial\Omega \setminus \partial_*\Omega) = 0$ and $\mathbb{C} \setminus \overline{\Omega}$ is also a* UR *domain with the same boundary as Ω.*

Moreover, the curve $\partial\Omega$ is rectifiable and, if L denotes its length and $[0, L] \ni s \mapsto z(s) \in \Sigma$ is its arc-length parametrization, then

$$\mathscr{H}^1(E) = \mathscr{L}^1(z^{-1}(E)) \quad \textit{for all measurable sets } E \subseteq \partial\Omega, \tag{2-63}$$

where $\mathscr{L}^1$ is the one-dimensional Lebesgue measure, and if ν denotes the geometric measure-theoretic outward unit normal to Ω then

$$\nu(z(s)) = -iz'(s) \quad \textit{for } \mathscr{L}^1\textit{-a.e. } s \in [0, L]. \tag{2-64}$$

A proof of Proposition 2.12 may be found in [Mitrea et al. 2016].

3. Background and preparatory estimates for singular integrals

The proofs of the main results require a number of prerequisites, and this section collects several useful estimates for singular integral operators. The first theorem in this regard essentially amounts to a version of the Calderón–Zygmund theory for singular integrals on uniformly rectifiable sets.

Theorem 3.1. *There exists a positive integer $N = N(n)$ with the following significance: Suppose $\Sigma \subseteq \mathbb{R}^n$ is a uniformly rectifiable set and define $\sigma := \mathcal{H}^{n-1}\lfloor\Sigma$. Also consider a complex-valued function*

$$k \in \mathscr{C}^N(\mathbb{R}^n \setminus \{0\}) \quad \textit{satisfying} \quad \begin{cases} k(-x) = -k(x) & \textit{for each } x \in \mathbb{R}^n, \\ k(\lambda\, x) = \lambda^{-(n-1)} k(x) & \textit{for all } \lambda > 0,\ x \in \mathbb{R}^n \setminus \{0\}. \end{cases} \tag{3-1}$$

For each $\varepsilon > 0$, consider the truncated singular integral operator

$$T_\varepsilon f(x) := \int_{\substack{y\in\Sigma \\ |x-y|>\varepsilon}} k(x-y) f(y)\, d\sigma(y), \quad x \in \Sigma, \tag{3-2}$$

and define the maximal operator T_* by setting

$$T_* f(x) := \sup_{\varepsilon>0} |T_\varepsilon f(x)|, \quad x \in \Sigma. \tag{3-3}$$

Then for each $p \in (1, \infty)$ there exists a constant $C \in (0, \infty)$, depending only on p and Σ, such that

$$\|T_* f\|_{L^p(\Sigma,\sigma)} \le C \|k|_{S^{n-1}}\|_{\mathscr{C}^N(S^{n-1})} \|f\|_{L^p(\Sigma,\sigma)} \tag{3-4}$$

for every $f \in L^p(\Sigma, \sigma)$. Furthermore, given any $p \in [1, \infty)$, for each function $f \in L^p(\Sigma, \sigma)$ the limit

$$Tf(x) := \lim_{\varepsilon\to 0^+} T_\varepsilon f(x) \tag{3-5}$$

exists for σ-a.e. $x \in \Sigma$, and the induced operators

$$T : L^p(\Sigma, \sigma) \longrightarrow L^p(\Sigma, \sigma), \quad p \in (1, \infty), \tag{3-6}$$

$$T : L^1(\Sigma, \sigma) \longrightarrow L^{1,\infty}(\Sigma, \sigma) \tag{3-7}$$

are well-defined, linear and bounded. In addition, for each $p \in (1, \infty)$, the adjoint of the operator T acting on $L^p(\Sigma, \sigma)$ is $-T$ acting on $L^{p'}(\Sigma, \sigma)$ with $1/p + 1/p' = 1$. Finally, corresponding to the endpoint $p = \infty$, the operator T also induces a linear and bounded mapping

$$T : L^\infty(\Sigma, \sigma) \longrightarrow \mathrm{BMO}(\Sigma). \tag{3-8}$$

Once the existence of the principal value singular integral operator T defined by the limit in (3-5) has been established, all other claims follow from [David and Semmes 1991] and standard harmonic analysis. As far as the issue of well-definedness of T is concerned, it is not difficult to reduce matters to the case when Σ is an $(n-1)$-dimensional Lipschitz graph (Taylor, personal communication, 2015). In the latter scenario, the desired result is known. For example, the desired conclusion is contained in [Hofmann et al. 2010, Theorem 3.33, p. 2669], where a more general result (applicable to variable coefficient operators on boundaries of UR domains) can be found. A direct proof for Lipschitz graphs may be found in [Hofmann et al. 2015, Proposition B.2, p. 163]. In this vein, see also [David 1991, pp. 63–64] for a sketch of a proof.

Our next theorem deals with nontangential maximal function estimates and jump relations for integral operators on UR domains. For a proof, the reader is once again referred to [Hofmann et al. 2010, Theorem 3.33, p. 2669].

Theorem 3.2. *Assume $\Omega \subset \mathbb{R}^n$ is a* UR *domain and let $\sigma := \mathcal{H}^{n-1}\lfloor\partial\Omega$ and ν denote the surface measure on $\partial\Omega$ and the outward unit normal to Ω, respectively. Select a function k as in* (3-1) *with $N = N(n)$ sufficiently large, and define*

$$\mathcal{T} f(x) := \int_{\partial\Omega} k(x-y) f(y)\, d\sigma(y), \quad x \in \Omega. \tag{3-9}$$

Then for each $p \in (1,\infty)$ there exists a finite constant $C = C(\Omega, k, p) > 0$ such that

$$\|\mathcal{N}(\mathcal{T} f)\|_{L^p(\partial\Omega,\sigma)} \le C\|f\|_{L^p(\partial\Omega,\sigma)} \quad \text{for all } f \in L^p(\partial\Omega,\sigma), \tag{3-10}$$

and, corresponding to $p = 1$,

$$\|\mathcal{N}(\mathcal{T} f)\|_{L^{1,\infty}(\partial\Omega,\sigma)} \le C\|f\|_{L^1(\partial\Omega,\sigma)} \quad \text{for all } f \in L^1(\partial\Omega,\sigma). \tag{3-11}$$

Also, if "hat" denotes the Fourier transform in $\mathbb{R}^n$ and $i := \sqrt{-1} \in \mathbb{C}$, then for every $f \in L^p(\partial\Omega,\sigma)$ with $p \in [1,\infty)$ the jump formula

$$(\mathcal{T} f\big|^{\rm nt}_{\partial\Omega})(x) = \lim_{\Gamma_\kappa \ni z \to x} \mathcal{T} f(z) = \frac{1}{2i}\hat{k}(\nu(x)) f(x) + Tf(x) \tag{3-12}$$

is valid at σ-a.e. point $x \in \partial\Omega$, where T is the principal value singular integral operator associated with the kernel k, as in (3-5).

The Fourier transform in $\mathbb{R}^n$ employed in (3-12) is

$$\hat{\phi}(\xi) := \int_{\mathbb{R}^n} e^{-i\langle x,\xi\rangle}\phi(x)\, dx, \quad \xi \in \mathbb{R}^n. \tag{3-13}$$

Let us also note that the hypotheses (3-1) imposed on the kernel k imply that $|k(x)| \le \|k\|_{L^\infty(S^{n-1})}|x|^{1-n}$ for each $x \in \mathbb{R}^n \setminus \{0\}$. Hence, k is a tempered distribution in $\mathbb{R}^n$ and $\hat{k}$, originally considered in the class of tempered distributions in $\mathbb{R}^n$, satisfies

$$\hat{k} \in \mathscr{C}^m(\mathbb{R}^n \setminus \{0\}) \text{ if } N \in \mathbb{N} \text{ is even and } m \in \mathbb{N}_0 \text{ is such that } m < N-1 \tag{3-14}$$

(see [Mitrea 2013, Exercise 4.60, p. 133]). In particular, (3-14) ensures that $\hat{k}(\nu(x))$ is meaningfully defined in (3-12) for σ-a.e. $x \in \partial\Omega$ whenever $N \ge 2$.

Lemma 3.3. *Suppose Ω is a nonempty, proper, open subset of $\mathbb{R}^n$ with a compact boundary, satisfying an upper Ahlfors regularity condition with constant $c \in (0,\infty)$. In this setting, define $\sigma := \mathcal{H}^{n-1}\lfloor\partial\Omega$ and consider an integral operator*

$$\mathscr{T} f(x) := \int_{\partial\Omega} k(x,y) f(y)\, d\sigma(y), \quad x \in \Omega, \tag{3-15}$$

whose kernel $k : \Omega \times \partial\Omega \to \mathbb{R}$ *has the property that there exists some finite positive constant* C_0 *such that*

$$|k(x, y)| \leq \frac{C_0}{|x-y|^{n-1}} \tag{3-16}$$

for each $x \in \Omega$ *and* σ*-a.e.* $y \in \partial\Omega$. *Also suppose that*

$$\sup_{x\in\Omega} |\mathscr{T}1(x)| < +\infty. \tag{3-17}$$

Then for every $\alpha \in (0, 1)$ *one has*

$$\sup_{x\in\Omega} |\mathscr{T}f(x)| \leq cC_0 \frac{2^{2n-2+\alpha}}{2^\alpha - 1}\big(1+[\operatorname{diam}(\partial\Omega)]^\alpha\big)[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} + \big(\|\mathscr{T}1\|_{L^\infty(\Omega)} + cC_0[\operatorname{diam}(\partial\Omega)]^{n-1}\big)\|f\|_{L^\infty(\partial\Omega)} \tag{3-18}$$

for every $f \in \mathscr{C}^\alpha(\partial\Omega)$.

Proof. Pick an arbitrary $f \in \mathscr{C}^\alpha(\partial\Omega)$ and fix any $x \in \Omega$. Consider first the case when $\operatorname{dist}(x, \partial\Omega) \geq 1$, in which we may directly estimate

$$|\mathscr{T}f(x)| \leq C_0\sigma(\partial\Omega)\|f\|_{L^\infty(\partial\Omega)} \leq cC_0[\operatorname{diam}(\partial\Omega)]^{n-1}\|f\|_{L^\infty(\partial\Omega)}. \tag{3-19}$$

In the case when $\operatorname{dist}(x, \partial\Omega) < 1$, select a point $x_* \in \partial\Omega$ such that

$$|x - x_*| = \operatorname{dist}(x, \partial\Omega) =: r \in (0, 1) \tag{3-20}$$

and split $\mathscr{T}f(x)$ into $I + II + III$, where

$$I := \int_{\partial\Omega\cap B(x_*,2r)} k(x, y)(f(y) - f(x_*))\, d\sigma(y), \tag{3-21}$$

$$II := \int_{\partial\Omega\setminus B(x_*,2r)} k(x, y)(f(y) - f(x_*))\, d\sigma(y), \tag{3-22}$$

$$III := (\mathscr{T}1)(x) f(x_*). \tag{3-23}$$

Note that

$$\begin{aligned} |I| &\leq \int_{\partial\Omega\cap B(x_*,2r)} |k(x, y)|\,|f(y) - f(x_*)|\, d\sigma(y) \\ &\leq C_0[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} \int_{\partial\Omega\cap B(x_*,2r)} \frac{|y-x_*|^\alpha}{|x-y|^{n-1}}\, d\sigma(y) \\ &\leq C_0[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} \frac{(2r)^\alpha}{r^{n-1}}\, \sigma(\partial\Omega \cap B(x_*, 2r)), \end{aligned} \tag{3-24}$$

where the third inequality comes from the facts that $|y - x_*|^\alpha \leq (2r)^\alpha$ on the domain of integration and that $1/|x - y| \leq 1/|x - x_*| = 1/r$ for all $y \in \partial\Omega$. Hence,

$$|I| \leq 2^{n-1+\alpha} cC_0[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)}, \tag{3-25}$$

bearing in mind (3-20) and the upper Ahlfors regularity of $\partial\Omega$. Also,

$$|II| \leq C_0[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} \int_{\partial\Omega\setminus B(x_*,2r)} \frac{|y-x_*|^\alpha}{|x-y|^{n-1}}\, d\sigma(y). \tag{3-26}$$

Note that if $y \in \partial\Omega \setminus B(x_*, 2r)$ then

$$|y-x_*| \leq |y-x| + |x-x_*| \quad \text{and} \quad r \leq \tfrac{1}{2}|y-x_*| \qquad \Longrightarrow \qquad |y-x_*| \leq 2|y-x|. \tag{3-27}$$

Hence, $1/|x-y|^{n-1} \leq 2^{n-1}/|y-x_*|^{n-1}$ on the domain of integration $\partial\Omega\setminus B(x_*, 2r)$. Also, if we introduce

$$N := \left[\log_2 \frac{\operatorname{diam}(\partial\Omega)}{r}\right] \in \mathbb{N}, \tag{3-28}$$

then $\partial\Omega \setminus B(x_*, 2^k r) = \varnothing$ for each integer $k > N$. Together, these observations and (3-26) allow us to estimate

$$\begin{aligned}
|II| &\leq 2^{n-1} C_0[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} \int_{\partial\Omega\setminus B(x_*,2r)} \frac{|y-x_*|^\alpha}{|y-x_*|^{n-1}}\, d\sigma(y) \\
&\leq 2^{n-1} C_0[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} \sum_{k=1}^{N} \int_{\partial\Omega\cap[B(x_*,2^{k+1}r)\setminus B(x_*,2^k r)]} \frac{1}{|y-x_*|^{n-1-\alpha}}\, d\sigma(y) \\
&\leq 2^{n-1} C_0[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} \sum_{k=1}^{N} (2^k r)^{-(n-1-\alpha)} \sigma(\partial\Omega \cap B(x_*, 2^{k+1} r)).
\end{aligned} \tag{3-29}$$

Thus, by the upper Ahlfors regularity condition,

$$\begin{aligned}
|II| &\leq 2^{n-1} C_0[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} \sum_{k=1}^{N} (2^k r)^{-(n-1-\alpha)} c(2^{k+1} r)^{n-1} \\
&= 2^{2n-2} c C_0 r^\alpha [f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} \sum_{k=1}^{N} (2^\alpha)^k \\
&\leq 2^{2n-2+\alpha} c C_0 r^\alpha [f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} \frac{(2^N)^\alpha}{2^\alpha - 1} \\
&\leq \frac{2^{2n-2+\alpha}}{2^\alpha - 1} c C_0 [f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} [\operatorname{diam}(\partial\Omega)]^\alpha.
\end{aligned} \tag{3-30}$$

Since, clearly, $|III| \leq \|\mathscr{T}1\|_{L^\infty(\Omega)} \|f\|_{L^\infty(\partial\Omega)}$, the desired conclusion follows. □

Lemma 3.4. *Retain the same assumptions on Ω as in Lemma 3.3 and consider an integral operator*

$$\mathscr{Q}f(x) := \int_{\partial\Omega} q(x,y) f(y)\, d\sigma(y), \quad x \in \Omega, \tag{3-31}$$

whose kernel $q : \Omega \times \partial\Omega \to \mathbb{R}$ is assumed to satisfy

$$|q(x,y)| \leq \frac{C_1}{|x-y|^n} \quad \textit{for all } x \in \Omega,\ y \in \partial\Omega, \tag{3-32}$$

for some finite positive constant C_1. *Also, with* ρ *as in* (2-56), *suppose there exists* $\alpha \in (0,1)$ *with the property that*

$$C_2 := \sup_{x\in\Omega}\big\{\rho(x)^{1-\alpha}|(\mathscr{Q}1)(x)|\big\} < +\infty. \tag{3-33}$$

Then one has

$$\sup_{x\in\Omega}\big\{\rho(x)^{1-\alpha}|\mathscr{Q}f(x)|\big\} \le \frac{2^{2n-1+\alpha}}{1-2^{\alpha-1}} cC_1[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} + C_2\|f\|_{L^\infty(\partial\Omega)} \tag{3-34}$$

for every $f \in \mathscr{C}^\alpha(\partial\Omega)$.

Proof. Select an arbitrary $f \in \mathscr{C}^\alpha(\partial\Omega)$. Pick some $x \in \Omega$ and choose $x_* \in \partial\Omega$ such that $|x-x_*| = \rho(x) =: r$. Split $\mathscr{Q}f(x)$ into $I + II + III$, where

$$I := \int_{\partial\Omega\cap B(x_*,2r)} q(x,y)[f(y)-f(x_*)]\,d\sigma(y), \tag{3-35}$$

$$II := \int_{\partial\Omega\setminus B(x_*,2r)} q(x,y)[f(y)-f(x_*)]\,d\sigma(y), \tag{3-36}$$

$$III := (\mathscr{Q}1)(x)f(x_*). \tag{3-37}$$

Then

$$\begin{aligned}
|I| &\le \int_{\partial\Omega\cap B(x_*,2r)} |q(x,y)|\,|f(y)-f(x_*)|\,d\sigma(y)\\
&\le C_1[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} \int_{\partial\Omega\cap B(x_*,2r)} \frac{|y-x_*|^\alpha}{|x-y|^n}\,d\sigma(y)\\
&\le C_1[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} \frac{(2r)^\alpha}{r^n}\sigma(\partial\Omega\cap B(x_*,2r)) \le 2^{n-1+\alpha}cC_1\rho(x)^{\alpha-1}[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)}.
\end{aligned} \tag{3-38}$$

Next, keeping in mind that $1/|x-y|^n \le 2^n/|y-x_*|^n$ on $\partial\Omega\setminus B(x_*,2r)$ (see (3-27)), we may estimate

$$\begin{aligned}
|II| &\le C_1[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} \int_{\partial\Omega\setminus B(x_*,2r)} \frac{|y-x_*|^\alpha}{|x-y|^n}\,d\sigma(y).\\
&\le 2^nC_1[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} \int_{\partial\Omega\setminus B(x_*,2r)} \frac{|y-x_*|^\alpha}{|y-x_*|^n}\,d\sigma(y)\\
&\le 2^nC_1[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} \sum_{k=1}^\infty \int_{\partial\Omega\cap[B(x_*,2^{k+1}r)\setminus B(x_*,2^kr)]} \frac{1}{|y-x_*|^{n-\alpha}}\,d\sigma(y)\\
&\le 2^nC_1[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} \sum_{k=1}^\infty (2^kr)^{-(n-\alpha)}\sigma(\partial\Omega\cap B(x_*,2^{k+1}r))\\
&\le 2^nC_1[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} \sum_{k=1}^\infty (2^kr)^{-(n-\alpha)}c(2^{k+1}r)^{n-1}\\
&= 2^{2n-1}cC_1r^{\alpha-1}[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} \sum_{k=1}^\infty (2^{\alpha-1})^k = \frac{2^{2n-2+\alpha}}{1-2^{\alpha-1}}cC_1\rho(x)^{\alpha-1}[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)}.
\end{aligned} \tag{3-39}$$

Given that $\rho(x)^{1-\alpha}|III| \le C_2\|f\|_{L^\infty(\partial\Omega)}$, the estimate (3-34) is established. □

Lemma 3.5. *Let Ω be a nonempty open proper subset of $\mathbb{R}^n$ whose boundary is compact and satisfies an upper Ahlfors regularity condition with constant $c \in (0, \infty)$. In this setting, define $\sigma := \mathcal{H}^{n-1}\lfloor\partial\Omega$ and consider an integral operator*

$$\mathcal{T}f(x) := \int_{\partial\Omega} K(x, y) f(y)\, d\sigma(y), \quad x \in \Omega, \tag{3-40}$$

whose kernel $K : \Omega \times \partial\Omega \to \mathbb{R}$ has the property that there exists a finite constant $B > 0$ such that

$$|K(x, y)| + |x - y|\,|\nabla_x K(x, y)| \le \frac{B}{|x - y|^{n-1}} \tag{3-41}$$

for each $x \in \Omega$ and σ-a.e. $y \in \partial\Omega$. Fix some $\alpha \in (0, 1)$ and suppose that

$$A := \sup_{x\in\Omega} |(\mathcal{T}1)(x)| + \sup_{x\in\Omega}\big\{\rho(x)^{1-\alpha}|\nabla(\mathcal{T}1)(x)|\big\} < +\infty. \tag{3-42}$$

Then for every $f \in \mathscr{C}^\alpha(\partial\Omega)$ one has

$$\begin{aligned}\sup_{x\in\Omega} |\mathcal{T}f(x)| + \sup_{x\in\Omega}\big\{\rho(x)^{1-\alpha}|\nabla(\mathcal{T}f)(x)|\big\} &\le cBC_{n,\alpha}\big(2 + [\mathrm{diam}(\partial\Omega)]^\alpha\big)[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)} \\ &\quad + \big(2A + cB[\mathrm{diam}(\partial\Omega)]^{n-1}\big)\|f\|_{L^\infty(\partial\Omega)},\end{aligned} \tag{3-43}$$

where

$$C_{n,\alpha} := 2^{2n-2-\alpha} \max\{(2^\alpha - 1)^{-1},\ 2(1 - 2^{\alpha-1})^{-1}\}. \tag{3-44}$$

As a consequence, there exists a finite constant $C_{n,\alpha,\Omega} > 0$ with the property that for every $f \in \mathscr{C}^\alpha(\partial\Omega)$ one has

$$\sup_{x\in\Omega} |\mathcal{T}f(x)| + \sup_{x\in\Omega}\big\{\rho(x)^{1-\alpha}|\nabla(\mathcal{T}f)(x)|\big\} \le C_{n,\alpha,\Omega}(A + B)\|f\|_{\mathscr{C}^\alpha(\partial\Omega)}. \tag{3-45}$$

Proof. This is an immediate consequence of Lemmas 3.3 and 3.4. □

4. Clifford analysis

A key tool for us is Clifford analysis, and here we elaborate on those aspects used in the proof of Theorem 1.1. To begin, the *Clifford algebra* with n imaginary units is the minimal enlargement of $\mathbb{R}^n$ to a unitary real algebra $(\mathcal{C}\ell_n, +, \odot)$ that is not generated (as an algebra) by any proper subspace of $\mathbb{R}^n$ and such that

$$x \odot x = -|x|^2 \quad \text{for any } x \in \mathbb{R}^n \hookrightarrow \mathcal{C}\ell_n. \tag{4-1}$$

This identity readily implies that, if $\{e_j\}_{1\le j\le n}$ is the standard orthonormal basis in $\mathbb{R}^n$, then

$$e_j \odot e_j = -1 \quad \text{and} \quad e_j \odot e_k = -e_k \odot e_j \quad \text{whenever } 1 \le j \ne k \le n. \tag{4-2}$$

In particular, identifying the canonical basis $\{e_j\}_{1\leq j\leq n}$ from $\mathbb{R}^n$ with the n imaginary units generating $\mathcal{C}\ell_n$, yields the embedding[4]

$$\mathbb{R}^n \hookrightarrow \mathcal{C}\ell_n, \quad \mathbb{R}^n \ni x = (x_1, \ldots, x_n) \equiv \sum_{j=1}^{n} x_j e_j \in \mathcal{C}\ell_n. \tag{4-3}$$

Also, any element $u \in \mathcal{C}\ell_n$ can be uniquely represented in the form

$$u = \sum_{l=0}^{n} {\sum_{|I|=l}}' u_I \, e_I, \quad u_I \in \mathbb{R}. \tag{4-4}$$

Here e_I stands for the product $e_{i_1} \odot e_{i_2} \odot \cdots \odot e_{i_l}$ if $I = (i_1, i_2, \ldots, i_l)$ and $e_0 := e_\varnothing := 1$ is the multiplicative unit. Also, $\sum'$ indicates that the sum is performed only over strictly increasing multi-indices, i.e., $I = (i_1, i_2, \ldots, i_l)$ with $1 \leq i_1 < i_2 < \cdots < i_l \leq n$. We endow $\mathcal{C}\ell_n$ with the natural Euclidean metric

$$|u| := \Big\{ \sum_I |u_I|^2 \Big\}^{\frac{1}{2}} \quad \text{for each } u = \sum_I u_I e_I \in \mathcal{C}\ell_n. \tag{4-5}$$

The Clifford conjugation on $\mathcal{C}\ell_n$, denoted by "bar", is defined as the unique real-linear involution on $\mathcal{C}\ell_n$ for which $\bar{e}_I e_I = e_I \bar{e}_I = 1$ for any multi-index I. More specifically, given $u = \sum_I u_I e_I \in \mathcal{C}\ell_n$ we set $\bar{u} := \sum_I u_I \bar{e}_I$ where, for each $I = (i_1, i_2, \ldots, i_l)$ with $1 \leq i_1 < i_2 < \cdots < i_l \leq n$,

$$\bar{e}_I = (-1)^l e_{i_l} \odot e_{i_{l-1}} \odot \cdots \odot e_{i_1}. \tag{4-6}$$

Let us also define the scalar part of $u = \sum_I u_I e_I \in \mathcal{C}\ell_n$ as $u_0 := u_\varnothing$, and endow $\mathcal{C}\ell_n$ with the natural Hilbert space structure

$$\langle u, v\rangle := \sum_I u_I v_I \quad \text{if } u = \sum_I u_I e_I, \; v = \sum_I v_I e_I \in \mathcal{C}\ell_n. \tag{4-7}$$

It follows directly from definitions that

$$\bar{x} = -x \quad \text{for each } x \in \mathbb{R}^n \hookrightarrow \mathcal{C}\ell_n, \tag{4-8}$$

and other properties are collected in the lemma below.

Lemma 4.1. *For any $u, v \in \mathcal{C}\ell_n$ one has*

$$|u|^2 = (u \odot \bar{u})_0 = (\bar{u} \odot u)_0, \tag{4-9}$$

$$\langle u, v\rangle = (u \odot \bar{v})_0 = (\bar{u} \odot v)_0, \tag{4-10}$$

$$\overline{u \odot v} = \bar{v} \odot \bar{u}, \tag{4-11}$$

[4]As the alert reader might have noted, for $n = 2$ the identification in (4-3) amounts to embedding $\mathbb{R}^2$ into the quaternions, i.e., $\mathbb{R}^2 \hookrightarrow \mathbb{H} := \{x_0 + x_1 \boldsymbol{i} + x_2 \boldsymbol{j} + x_3 \boldsymbol{k} : x_0, x_1, x_2, x_3 \in \mathbb{R}\}$ via $(x_1, x_2) \equiv x_1 \boldsymbol{i} + x_2 \boldsymbol{j} \in \mathbb{H}$. The reader is reassured that this is simply a matter of convenience, and we might as well have arranged that the embedding (4-3) comes down, when $n = 2$, to perhaps the more familiar identification $\mathbb{R}^2 \equiv \mathbb{C}$, by taking $x = (x_0, x_1, \ldots, x_{n-1}) \equiv x_0 + x_1 e_1 + \ldots x_{n-1} e_{n-1} \in \mathcal{C}\ell_{n-1}$. The latter choice leads to a parallel theory to the one presented here, entailing only minor natural alterations.

$$|\overline{u}| = |u|, \tag{4-12}$$

$$|u \odot v| \leq 2^{n/2}|u||v|, \tag{4-13}$$

and

$$|u \odot v| = |u||v| \quad \text{if either } u \text{ or } v \text{ belongs to } \mathbb{R}^n \hookrightarrow \mathcal{C}\ell_n. \tag{4-14}$$

Proof. Properties (4-9)–(4-12) are straightforward consequences of the definitions. To justify (4-13), assume $u = \sum_I u_I e_I \in \mathcal{C}\ell_n$ and $v = \sum_J v_J e_J \in \mathcal{C}\ell_n$ have been given. Then

$$\begin{aligned}|u \odot v| = \Big|\sum_I \Big(\sum_J u_I v_J e_I \odot e_J\Big)\Big| \leq \sum_I \Big|\sum_J u_I v_J e_I \odot e_J\Big| = \sum_I \Big(\sum_J |u_I v_J|^2\Big)^{\frac{1}{2}} = |v| \sum_I |u_I| \\ \leq |v|\Big(\sum_I |u_I|^2\Big)^{\frac{1}{2}}\Big(\sum_I 1\Big)^{\frac{1}{2}} = 2^{n/2}|u||v|.\end{aligned} \tag{4-15}$$

Above, the triangle inequality has been employed in the second step. The third step relies on (4-5) and the observation that, for each fixed I, the family of Clifford algebra elements $\{e_I \odot e_J\}_J$ coincides modulo signs with the orthonormal basis $\{e_K\}_K$. The penultimate step is the discrete Cauchy–Schwarz inequality.

As regards (4-14), assume that $v \in \mathbb{R}^n \hookrightarrow \mathcal{C}\ell_n$ and write

$$|u \odot v|^2 = ((u \odot v) \odot \overline{u \odot v})_0 = (u \odot (v \odot \overline{v}) \odot \overline{u})_0 = |v|^2 (u \odot \overline{u})_0 = |u|^2|v|^2, \tag{4-16}$$

by (4-9), (4-11), (4-8) and (4-1). Finally, the case when $u \in \mathbb{R}^n \hookrightarrow \mathcal{C}\ell_n$ follows from what we have just proved, with the help of (4-11) and (4-12). □

Next, recall the *Dirac operator*

$$D := \sum_{j=1}^n e_j \partial_j. \tag{4-17}$$

In the sequel, we shall use D_L and D_R to denote the action of D on a $\mathscr{C}^1$ function $u : \Omega \to \mathcal{C}\ell_n$ (where Ω is an open subset of $\mathbb{R}^n$) from the left and from the right, respectively. For a sufficiently nice domain Ω with outward unit normal $\nu = (\nu_1, \dots, \nu_n)$ — identified with the $\mathcal{C}\ell_n$-valued function $\nu = \sum_{j=1}^n \nu_j e_j$ — and surface measure σ, and for any two reasonable $\mathcal{C}\ell_n$-valued functions u and v in Ω, the following integration by parts formula holds:

$$\int_{\partial\Omega} u(x) \odot \nu(x) \odot v(x)\, d\sigma(x) = \int_\Omega \big((D_R u)(x) \odot v(x) + u(x) \odot (D_L v)(x)\big)\, dx. \tag{4-18}$$

More detailed accounts of these and related matters can be found in [Brackx et al. 1982; Mitrea 1994]. In general, if $(\mathscr{X}, \|\cdot\|_{\mathscr{X}})$ is a Banach space then by $\mathscr{X} \otimes \mathcal{C}\ell_n$ we shall denote the Banach space consisting of elements of the form

$$u = \sum_{l=0}^n {\sum_{|I|=l}}' u_I\, e_I, \quad u_I \in \mathscr{X}, \tag{4-19}$$

equipped with the natural norm

$$\|u\|_{\mathscr{X}\otimes\mathcal{C}\ell_n} := \sum_{l=0}^{n} {\sum_{|I|=l}}' \|u_I\|_{\mathscr{X}}. \tag{4-20}$$

A simple but useful observation in this context is that:

> If $\Omega \subset \mathbb{R}^n$ is a domain of class $\mathscr{C}^{1+\alpha}$ for some $\alpha \in (0,1)$ then $\nu\odot$: $\mathscr{C}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n \to \mathscr{C}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n$ is an isomorphism whose norm and the norm of its inverse are at most $2\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)}$. (4-21)

Indeed, by (4-1), its inverse is $-\nu\odot$ and the aforementioned norm estimates are simple consequences of (4-14), bearing in mind that $\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)} \geq 1$.

For each $s \in \{1,\dots,n\}$ we let $[\,\cdot\,]_s$ denote the projection onto the s-th Euclidean coordinate, i.e., $[x]_s := x_s$ if $x = (x_1,\dots,x_n) \in \mathbb{R}^n$. The following lemma, in the spirit of work of Semmes [1989], will play an important role for us.

Lemma 4.2. *For any odd, harmonic, homogeneous polynomial $P(x)$, $x \in \mathbb{R}^n$ (with $n \geq 2$), of degree $l \geq 3$, there exist a family $P_{rs}(x)$, $1 \leq r, s \leq n$, of harmonic, homogeneous polynomials of degree $l-2$, as well as a family of odd $\mathscr{C}^\infty$ functions*

$$k_{rs} : \mathbb{R}^n \setminus \{0\} \longrightarrow \mathbb{R}^n \hookrightarrow \mathcal{C}\ell_n, \quad 1 \leq r, s \leq n, \tag{4-22}$$

which are homogeneous of degree $-(n-1)$ and, for each $x \in \mathbb{R}^n \setminus \{0\}$, satisfy

$$\frac{P(x)}{|x|^{n-1+l}} = \sum_{r,s=1}^{n} [k_{rs}(x)]_s, \tag{4-23}$$

$$(D_R k_{rs})(x) = \frac{l-1}{n+l-3}\frac{\partial}{\partial x_r}\left(\frac{P_{rs}(x)}{|x|^{n+l-3}}\right), \quad 1 \leq r, s \leq n. \tag{4-24}$$

Moreover, there exists a finite-dimensional constant $c_n > 0$ such that

$$\max_{1\leq r,s\leq n} \|k_{rs}\|_{L^\infty(S^{n-1})} + \max_{1\leq r,s\leq n} \|\nabla k_{rs}\|_{L^\infty(S^{n-1})} \leq c_n\, 2^l \|P\|_{L^1(S^{n-1})}. \tag{4-25}$$

Proof. Given an odd, harmonic, homogeneous polynomial $P(x)$ of degree $l \geq 3$ in $\mathbb{R}^n$, for $r, s \in \{1,\dots,n\}$ introduce

$$P_{rs}(x) := \frac{1}{l(l-1)}(\partial_r\partial_s P)(x) \quad \text{for all } x \in \mathbb{R}^n. \tag{4-26}$$

Then each P_{rs} is an odd, harmonic, homogeneous polynomial of degree $l-2$ in $\mathbb{R}^n$, and Euler's formula for homogeneous functions gives

$$P(x) = \sum_{r,s=1}^{n} x_r x_s P_{rs}(x) \quad \text{for all } x \in \mathbb{R}^n \tag{4-27}$$

and, for each $r, s \in \{1,\dots,n\}$,

$$\langle(\nabla P_{rs})(x), x\rangle = (l-2)P_{rs}(x) \quad \text{for all } x \in \mathbb{R}^n. \tag{4-28}$$

To proceed, assume first that $n \geq 3$ and define the function $k_{rs} : \mathbb{R}^n \setminus \{0\} \longrightarrow \mathbb{R}^n \hookrightarrow \mathcal{C}\ell_n$ for each $r, s \in \{1, \dots, n\}$ by setting

$$k_{rs}(x) := \frac{1}{(n+l-3)(n+l-5)} \sum_{j=1}^{n} \partial_r \partial_j \left(\frac{P_{rs}(x)}{|x|^{n+l-5}} \right) e_j \quad \text{for all } x \in \mathbb{R}^n \setminus \{0\}. \tag{4-29}$$

The fact that $n, l \geq 3$ ensures that both $n+l-3 \neq 0$ and $n+l-5 \neq 0$, so each k_{rs} is well-defined, odd, $\mathscr{C}^\infty$ and homogeneous of degree $-(n-1)$ in $\mathbb{R}^n \setminus \{0\}$. In addition,

$$k_{rs}(x) = \frac{1}{(n+l-3)(n+l-5)} D_R \left[\partial_r \left(\frac{P_{rs}(x)}{|x|^{n+l-5}} \right) \right] \quad \text{for all } x \in \mathbb{R}^n \setminus \{0\}; \tag{4-30}$$

hence, for all $x \in \mathbb{R}^n \setminus \{0\}$ we may write

$$\begin{aligned} (D_R k_{rs})(x) &= \frac{1}{(n+l-3)(n+l-5)} D_R^2 \left[\partial_r \left(\frac{P_{rs}(x)}{|x|^{n+l-5}} \right) \right] \\ &= \frac{-1}{(n+l-3)(n+l-5)} \Delta \left[\partial_r \left(\frac{P_{rs}(x)}{|x|^{n+l-5}} \right) \right] \\ &=: I + II + III, \end{aligned} \tag{4-31}$$

where

$$\begin{aligned} I &:= \frac{-1}{(n+l-3)(n+l-5)} \partial_r \left[\frac{(\Delta P_{rs})(x)}{|x|^{n+l-5}} \right] = 0, \\ II &:= \frac{-1}{(n+l-3)(n+l-5)} \partial_r \left[2 \langle (\nabla P_{rs})(x), \nabla [|x|^{-(n+l-5)}] \rangle \right] \\ &= \frac{2}{n+l-3} \partial_r \left[\frac{\langle (\nabla P_{rs})(x), x \rangle}{|x|^{n+l-3}} \right] = \frac{2(l-2)}{n+l-3} \partial_r \left[\frac{P_{rs}(x)}{|x|^{n+l-3}} \right], \\ III &:= \frac{-1}{(n+l-3)(n+l-5)} \partial_r \left[P_{rs}(x) \Delta [|x|^{-(n+l-5)}] \right] = \frac{-l+3}{n+l-3} \partial_r \left[\frac{P_{rs}(x)}{|x|^{n+l-3}} \right], \end{aligned} \tag{4-32}$$

by the harmonicity of P, (4-28), and straightforward algebra. This proves that (4-23) holds when $n \geq 3$. Going further, from (4-29) and the fact that

$$\sum_{r=1}^{n} (\partial_r P_{rs})(x) = \sum_{s=1}^{n} (\partial_s P_{rs})(x) = 0 \quad \text{and} \quad \sum_{r=1}^{n} P_{rr}(x) = 0 \tag{4-33}$$

(as seen from (4-26) and the harmonicity of P), we deduce that, for each $x \in \mathbb{R}^n \setminus \{0\}$,

$$\begin{aligned} \sum_{r,s=1}^{n} [k_{rs}(x)]_s &= \frac{1}{(n+l-3)(n+l-5)} \sum_{r,s=1}^{n} \partial_r \partial_s \left(\frac{P_{rs}(x)}{|x|^{n+l-5}} \right) \\ &= \frac{1}{(n+l-3)(n+l-5)} \sum_{r,s=1}^{n} P_{rs}(x) \partial_r \partial_s [|x|^{-(n+l-5)}] \\ &= \frac{-1}{n+l-3} \sum_{r,s=1}^{n} P_{rs}(x) \left\{ \frac{\delta_{rs}}{|x|^{n+l-3}} - (n+l-3) \frac{x_r x_s}{|x|^{n+l-1}} \right\} = \frac{P(x)}{|x|^{n-1+l}}. \end{aligned} \tag{4-34}$$

This establishes (4-24) for $n \geq 3$. Moving on, for each $\gamma \in \mathbb{N}_0^n$, interior estimates for the harmonic function P give

$$\|\partial^\gamma P\|_{L^\infty(S^{n-1})} \leq c_{n,\gamma} \int_{B(0,2)} |P(x)|\,dx = c_{n,\gamma} \int_{S^{n-1}} |P(\omega)| \biggl(\int_0^2 r^{n-1+l}\,dr \biggr) d\omega = c_{n,\gamma} \frac{2^l}{n+l} \|P\|_{L^1(S^{n-1})}, \tag{4-35}$$

where we have also used the fact that P is homogeneous of degree l. The estimates in (4-25) now readily follow on account of (4-29), (4-26), and (4-35).

To treat the two-dimensional case, first we observe that, if $Q_m(x)$ is an arbitrary homogeneous polynomial of degree $m \in \mathbb{N}_0$ in $\mathbb{R}^n$ with $n \geq 2$ and $\lambda > 0$, then

$$\frac{Q_m(x)}{|x|^{n+m-\lambda}} \quad \text{is a tempered distribution in } \mathbb{R}^n. \tag{4-36}$$

If, in addition, $Q_m(x)$ is harmonic and $\lambda < n$ then (see [Stein 1970, p. 73]) also

$$\mathcal{F}_{x\to\xi}\biggl(\frac{Q_m(x)}{|x|^{n+m-\lambda}}\biggr) = \gamma_{n,m,\lambda} \frac{Q_m(\xi)}{|\xi|^{m+\lambda}} \quad \text{as tempered distributions in } \mathbb{R}^n, \tag{4-37}$$

where $\mathcal{F}_{x\to\xi}$ is an alternative notation for the Fourier transform in $\mathbb{R}^n$ from (3-13) and

$$\gamma_{n,m,\lambda} := (-1)^{3m/2} \pi^{n/2} 2^\lambda \frac{\Gamma(m/2+\lambda/2)}{\Gamma(m/2+n/2-\lambda/2)}. \tag{4-38}$$

Now pick an odd, harmonic, homogeneous polynomial $P(x)$ of degree $l \geq 3$ in $\mathbb{R}^2$ and define P_{rs} for r, $s \in \{1, \dots, n\}$ as in (4-26). Hence, once again, each P_{rs} is an odd, harmonic, homogeneous polynomial of degree $l-2$ in $\mathbb{R}^2$, and (4-27) holds. Moreover, (4-37) used for $n=2$, $m=l-2$, $\lambda=1$ and $Q_m = P_{rs}$ yields

$$\frac{P_{rs}(x)}{|x|^{l-1}} = -(-1)^{3l/2} 2\pi \mathcal{F}^{-1}_{\xi\to x}\biggl(\frac{P_{rs}(\xi)}{|\xi|^{l-1}}\biggr). \tag{4-39}$$

Now, for each r, $s \in \{1, 2\}$ define the function $k_{rs} : \mathbb{R}^2 \setminus \{0\} \longrightarrow \mathbb{R}^2 \hookrightarrow \mathcal{C}\ell_2$ by setting

$$k_{rs}(x) := (-1)^{3l/2} 2\pi \sum_{j=1}^{2} \mathcal{F}^{-1}_{\xi\to x}\biggl(\xi_r \xi_j \frac{P_{rs}(\xi)}{|\xi|^{l+1}}\biggr) e_j \quad \text{for all } x \in \mathbb{R}^2 \setminus \{0\}. \tag{4-40}$$

By (4-36) used with $n=2$, $m=l$, $\lambda=1$ and $Q_m(\xi) = \xi_r \xi_j P_{rs}(\xi)$, it follows that $\xi_r \xi_j P_{rs}(\xi)/|\xi|^{l+1}$ is a tempered distribution in $\mathbb{R}^2$. Consequently, k_{rs} in (4-40) is meaningfully defined and, from [Mitrea 2013, Proposition 4.58, p. 132], we deduce that $k_{rs} \in \mathscr{C}^\infty(\mathbb{R}^2 \setminus \{0\})$. Also, based on standard properties of the Fourier transform (see, e.g., [Mitrea 2013, Chapter 4]) it follows that k_{rs} is odd and homogeneous of degree -1 in $\mathbb{R}^2 \setminus \{0\}$. In addition,

$$\begin{aligned}(D_R k_{rs})(x) &= (-1)^{3l/2} 2\pi \sum_{\ell,j=1}^{2} \partial_{x_\ell} \mathcal{F}^{-1}_{\xi\to x}\biggl(\xi_r \xi_j \frac{P_{rs}(\xi)}{|\xi|^{l+1}}\biggr) e_j \odot e_\ell \\ &= \sqrt{-1}(-1)^{3l/2} 2\pi \sum_{\ell,j=1}^{2} \mathcal{F}^{-1}_{\xi\to x}\biggl(\xi_r \xi_j \xi_\ell \frac{P_{rs}(\xi)}{|\xi|^{l+1}}\biggr) e_j \odot e_\ell =: I + II,\end{aligned} \tag{4-41}$$

where I and II are the pieces produced by summing up over $j=\ell$ and $j\neq\ell$, respectively. Since, in the latter scenario, $\xi_\ell\xi_j=\xi_j\xi_\ell$ while $e_j\odot e_\ell=-e_\ell\odot e_j$, it follows that $II=0$. Given that $e_j\odot e_j=-1$ for each $j\in\{1,2\}$, we conclude that

$$\begin{aligned}(D_R k_{rs})(x)&=-\sqrt{-1}(-1)^{3l/2}2\pi\sum_{j=1}^{2}\mathcal{F}^{-1}_{\xi\to x}\biggl(\xi_r\xi_j^2\frac{P_{rs}(\xi)}{|\xi|^{l+1}}\biggr)\\&=-\sqrt{-1}(-1)^{3l/2}2\pi\mathcal{F}^{-1}_{\xi\to x}\biggl(\xi_r\frac{P_{rs}(\xi)}{|\xi|^{l-1}}\biggr)\\&=-(-1)^{3l/2}2\pi\,\partial_{x_r}\biggl[\mathcal{F}^{-1}_{\xi\to x}\biggl(\frac{P_{rs}(\xi)}{|\xi|^{l-1}}\biggr)\biggr]=\partial_{x_r}\biggl[\frac{P_{rs}(x)}{|x|^{l-1}}\biggr],\end{aligned}\tag{4-42}$$

where the last step uses (4-39). Hence, (4-23) holds when $n=2$. Finally, from (4-29), (4-27) and (4-37) (used for P) we deduce that for each $x\in\mathbb{R}^2\setminus\{0\}$ we have

$$\sum_{r,s=1}^{2}[k_{rs}(x)]_s=(-1)^{3l/2}2\pi\sum_{r,s=1}^{2}\mathcal{F}^{-1}_{\xi\to x}\biggl(\xi_r\xi_s\frac{P_{rs}(\xi)}{|\xi|^{l+1}}\biggr)=(-1)^{3l/2}2\pi\mathcal{F}^{-1}_{\xi\to x}\biggl(\frac{P(\xi)}{|\xi|^{l+1}}\biggr)=\frac{P(x)}{|x|^{l+1}}.\tag{4-43}$$

This establishes (4-24) when $n=2$.

At this stage, it remains to justify (4-25) in the case $n=2$. To this end, pick $\psi\in\mathscr{C}_0^\infty(\mathbb{R}^2)$ with $0\le\psi\le 1$, $\psi=1$ on $B(0,1)$ and $\psi=0$ on $\mathbb{R}^2\setminus\overline{B(0,2)}$. Fix $r,s,j\in\{1,2\}$ and abbreviate $u(\xi):=\xi_r\xi_j P_{rs}(\xi)/|\xi|^{l+1}$ for $\xi\in\mathbb{R}^2\setminus\{0\}$. Then u is locally integrable and defines a tempered distribution in $\mathbb{R}^2$. Hence, for each $\alpha\in\mathbb{N}_0^2$ with $|\alpha|=2$ and $\xi\in\overline{B(0,1)}$ we may write

$$\begin{aligned}|\mathcal{F}_{x\to\xi}(\psi(x)\partial^\alpha u(x))|&=|\langle\psi\partial^\alpha u,e^{-i\langle\xi,\cdot\rangle}\rangle|=|\langle u,\partial^\alpha(\psi e^{-i\langle\xi,\cdot\rangle})\rangle|\\&\le C\int_{B(0,2)}|u(x)|\,dx\le C\int_{S^1}|P_{rs}(\omega)|\,d\omega\le C2^l\|P\|_{L^1(S^1)}\end{aligned}\tag{4-44}$$

and

$$\begin{aligned}\bigl|\mathcal{F}_{x\to\xi}\bigl((1-\psi(x))\partial^\alpha u(x)\bigr)\bigr|&\le\|(1-\psi)\partial^\alpha u\|_{L^1(\mathbb{R}^2)}\le\int_{\mathbb{R}^2\setminus B(0,1)}|\partial^\alpha u(x)|\,dx\\&\le C\int_{S^1}|\partial^\alpha u(\omega)|\,d\omega\le C2^l\|P\|_{L^1(S^1)}.\end{aligned}\tag{4-45}$$

Collectively, (4-44) and (4-45) give that, for each $\alpha\in\mathbb{N}_0^2$ with $|\alpha|=2$ and $\xi\in\overline{B(0,1)}$,

$$|\mathcal{F}_{x\to\xi}(\partial^\alpha u(x))|\le|\mathcal{F}_{x\to\xi}(\psi(x)\partial^\alpha u(x))|+\bigl|\mathcal{F}_{x\to\xi}\bigl((1-\psi(x))\partial^\alpha u(x)\bigr)\bigr|\le C2^l\|P\|_{L^1(S^1)};\tag{4-46}$$

hence, for each $\xi\in\overline{B(0,1)}$ we have

$$|\xi|^2|\hat{u}(\xi)|=\sum_{\ell=1}^{2}|\xi_\ell^2\hat{u}(\xi)|=\sum_{\ell=1}^{2}|\mathcal{F}_{x\to\xi}(\partial_\ell^2 u(x))|\le C2^l\|P\|_{L^1(S^1)}.\tag{4-47}$$

In particular, $\|k_{rs}\|_{L^\infty(S^1)}\le C\sup_{|\xi|=1}|\hat{u}(\xi)|\le C2^l\|P\|_{L^1(S^1)}$. A similar combination of ideas also yields $\|\nabla k_{rs}\|_{L^\infty(S^1)}\le C2^l\|P\|_{L^1(S^1)}$. This proves (4-25) in the case $n=2$ and completes the proof of the lemma. □

5. Cauchy–Clifford operators on Hölder spaces

Let $\Omega \subset \mathbb{R}^n$ be a set of locally finite perimeter satisfying (2-16). As before, we shall denote by $\nu = (\nu_1, \dots, \nu_n)$ the outward unit normal to Ω and by $\sigma := \mathcal{H}^{n-1} \lfloor \partial\Omega$ the surface measure on $\partial\Omega$. Then the (boundary-to-domain) *Cauchy–Clifford operator* and its principal value (or boundary-to-boundary) version associated with Ω are, respectively, given by

$$\mathcal{C} f(x) := \frac{1}{\omega_{n-1}} \int_{\partial\Omega} \frac{x-y}{|x-y|^n} \odot \nu(y) \odot f(y)\, d\sigma(y), \quad x \in \Omega, \tag{5-1}$$

and

$$\mathcal{C}^{\mathrm{pv}} f(x) := \lim_{\varepsilon \to 0^+} \frac{1}{\omega_{n-1}} \int_{\substack{y \in \partial\Omega \\ |x-y| > \varepsilon}} \frac{x-y}{|x-y|^n} \odot \nu(y) \odot f(y)\, d\sigma(y), \quad x \in \partial\Omega, \tag{5-2}$$

where f is a $\mathcal{C}\ell_n$-valued function defined on $\partial\Omega$. At the present time, these definitions are informal as more conditions need to be imposed on the function f and the underlying domain Ω in order to ensure that these operators are well-defined and enjoy desirable properties in various settings of interest. We start by recording the following result, in the context of uniformly rectifiable domains.

Proposition 5.1. *Let $\Omega \subset \mathbb{R}^n$ be a* UR *domain. Then, for every $f \in L^p(\partial\Omega, \sigma) \otimes \mathcal{C}\ell_n$ with $p \in [1, \infty)$, the function $\mathcal{C}^{\mathrm{pv}} f$ is meaningfully defined σ-a.e. on $\partial\Omega$, and the actions of the two Cauchy–Clifford operators on f are related via the boundary behavior*

$$(\mathcal{C} f\big|^{\mathrm{nt}}_{\partial\Omega})(x) := \lim_{\substack{z \to x \\ z \in \Gamma_\kappa(x)}} \mathcal{C} f(z) = \big(\tfrac{1}{2} I + \mathcal{C}^{\mathrm{pv}}\big) f(x) \quad \text{for } \sigma\text{-a.e. } x \in \partial\Omega, \tag{5-3}$$

where I is the identity operator. Moreover, for each $p \in (1, \infty)$, there exists a finite constant $M = M(n, p, \Omega) > 0$ such that

$$\|\mathcal{N}(\mathcal{C} f)\|_{L^p(\partial\Omega,\sigma)} \le M \|f\|_{L^p(\partial\Omega,\sigma)\otimes\mathcal{C}\ell_n}, \tag{5-4}$$

the operator $\mathcal{C}^{\mathrm{pv}}$ is well-defined and bounded on $L^p(\partial\Omega, \sigma) \otimes \mathcal{C}\ell_n$, and the formula

$$(\mathcal{C}^{\mathrm{pv}})^2 = \tfrac{1}{4} I \quad \text{on } L^p(\partial\Omega, \sigma) \otimes \mathcal{C}\ell_n \tag{5-5}$$

holds.

Proof. With the exception of (5-5) (which has been proved in [Hofmann et al. 2010]; see also [Mitrea et al. 2015] for very general results of this type), all claims follow from Theorems 3.1–3.2. □

The goal in this section is to prove similar results when the Lebesgue scale is replaced by Hölder spaces, in a class of domains considerably more general than the category of uniformly rectifiable domains. We begin by proving the following result:

Lemma 5.2. *Let $\Omega \subseteq \mathbb{R}^n$ be a Lebesgue measurable set whose boundary is compact and upper Ahlfors regular* (*hence, in particular, Ω is of locally finite perimeter by* (2-22)). *Denote by ν the geometric measure-theoretic outward unit normal to Ω and define $\sigma := \mathcal{H}^{n-1} \lfloor \partial_* \Omega$. Then there exists a number*

$N = N(n, c) \in (0, \infty)$, *depending only on the dimension* n *and the upper Ahlfors regularity constant* c *of* $\partial\Omega$, *with the property that*

$$\left| \int_{\partial_*\Omega \setminus B(x,r)} \frac{x-y}{|x-y|^n} \odot \nu(y)\, d\sigma(y) \right| \le N \quad \textit{for all } x \in \mathbb{R}^n,\ r \in (0,\infty). \tag{5-6}$$

Proof. We shall first show that, whenever $\Omega \subseteq \mathbb{R}^n$ is a bounded set of locally finite perimeter, having fixed an arbitrary $x \in \mathbb{R}^n$, for $\mathscr{L}^1$-a.e. $\varepsilon > 0$ we have

$$\int_{\partial_*\Omega \setminus B(x,\varepsilon)} \frac{x-y}{|x-y|^n} \odot \nu(y)\, d\sigma(y) = \int_{\Omega \cap \partial B(x,\varepsilon)} \frac{x-y}{|x-y|^n} \odot \nu(y)\, d\mathcal{H}^{n-1}(y) = \frac{\mathcal{H}^{n-1}(\Omega \cap \partial B(x,\varepsilon))}{\varepsilon^{n-1}}. \tag{5-7}$$

To justify this claim, we start by noting that the second equality (which holds for any measurable set $\Omega \subset \mathbb{R}^n$) is an immediate consequence of the fact that

$$y \in \partial B(x,\varepsilon) \implies (x-y) \odot \nu(y) = (x-y) \odot (y-x)/\varepsilon = \varepsilon. \tag{5-8}$$

As regards the first equality in (5-7), for each $j, k \in \{1, \dots, n\}$ consider the vector field

$$\vec{F}_{jk}(y) := \left(0, \dots, 0, \frac{x_j - y_j}{|x-y|^n}, 0, \dots, 0\right) \quad \text{for all } y \in \mathbb{R}^n \setminus \{x\}, \tag{5-9}$$

with the nonzero component on the k-th slot. Thus, we have $\vec{F}_{jk} \in \mathscr{C}^1(\mathbb{R}^n \setminus \{x\}, \mathbb{R}^n)$ and, if E_Δ stands for the standard fundamental solution for the Laplacian $\Delta = \partial_1^2 + \cdots \partial_n^2$ in $\mathbb{R}^n$, given by

$$E_\Delta(x) := \begin{cases} \dfrac{1}{\omega_{n-1}(2-n)} \dfrac{1}{|x|^{n-2}} & \text{if } n \ge 3, \\ \dfrac{1}{2\pi} \ln|x| & \text{if } n = 2, \end{cases} \qquad \text{for all } x \in \mathbb{R}^n \setminus \{0\}, \tag{5-10}$$

then

$$(\operatorname{div} \vec{F}_{jk})(y) = -\omega_{n-1}(\partial_j \partial_k E_\Delta)(x-y) \quad \text{for all } y \in \mathbb{R}^n \setminus \{x\}. \tag{5-11}$$

As a consequence, in $\mathbb{R}^n \setminus \{x\}$ we have

$$\begin{aligned} \sum_{j,k=1}^n (\operatorname{div} \vec{F}_{jk}) e_j \odot e_k &= \sum_{1 \le j \ne k \le n} (\operatorname{div} \vec{F}_{jk}) e_j \odot e_k - \sum_{j=1}^n \operatorname{div} \vec{F}_{jj} \\ &= -\omega_{n-1} \sum_{1 \le j \ne k \le n} (\partial_j \partial_k E_\Delta)(x - \cdot) e_j \odot e_k + \omega_{n-1}(\Delta E_\Delta)(x - \cdot) \\ &= 0, \end{aligned} \tag{5-12}$$

using the fact that $e_j \odot e_k = -e_k \odot e_j$ for $j \ne k$ and the harmonicity of $E_\Delta(x - \cdot)$ in $\mathbb{R}^n \setminus \{x\}$.

At this stage, fix an arbitrary $\varepsilon_o \in (0, \infty)$ and alter each $\vec{F}_{jk}$ both inside $B(x, \varepsilon_o)$ and outside an open neighborhood of $\overline{\Omega}$ to a vector field $\vec{G}_{jk} \in \mathscr{C}_0^1(\mathbb{R}^n, \mathbb{R}^n)$ (this is possible given the working assumption that Ω is bounded). Then, for $\mathscr{L}^1$-a.e. $\varepsilon \in (\varepsilon_o, \infty)$, based on the formula (2-62) used for $\vec{F} := \vec{G}_{jk}$, $D := \Omega$

and $r := \varepsilon$ we may write

$$\begin{aligned}
0 &= \sum_{j,k=1}^{n}\Big(\int_{\Omega\setminus B(x,\varepsilon)} \operatorname{div}\vec{F}_{jk}\,d\mathscr{L}^n\Big)e_j\odot e_k = \sum_{j,k=1}^{n}\Big(\int_{\Omega\setminus B(x,\varepsilon)} \operatorname{div}\vec{G}_{jk}\,d\mathscr{L}^n\Big)e_j\odot e_k\\
&= \sum_{j,k=1}^{n}\Big(\int_{\partial_*\Omega\setminus B(x,\varepsilon)} \langle\vec{G}_{jk},\nu\rangle\,d\sigma\Big)e_j\odot e_k - \sum_{j,k=1}^{n}\Big(\int_{\Omega\cap\partial B(x,\varepsilon)} \langle\vec{G}_{jk},\nu\rangle\,d\mathcal{H}^{n-1}\Big)e_j\odot e_k\\
&= \sum_{j,k=1}^{n}\Big(\int_{\partial_*\Omega\setminus B(x,\varepsilon)} \langle\vec{F}_{jk},\nu\rangle\,d\sigma\Big)e_j\odot e_k - \sum_{j,k=1}^{n}\Big(\int_{\Omega\cap\partial B(x,\varepsilon)} \langle\vec{F}_{jk},\nu\rangle\,d\mathcal{H}^{n-1}\Big)e_j\odot e_k\\
&= \sum_{j,k=1}^{n}\Big(\int_{\partial_*\Omega\setminus B(x,\varepsilon)} \frac{(x_j-y_j)\nu_k(y)}{|x-y|^n}\,d\sigma(y)\Big)e_j\odot e_k\\
&\qquad\qquad - \sum_{j,k=1}^{n}\Big(\int_{\Omega\cap\partial B(x,\varepsilon)} \frac{(x_j-y_j)\nu_k(y)}{|x-y|^n}\,d\mathcal{H}^{n-1}(y)\Big)e_j\odot e_k\\
&= \int_{\partial_*\Omega\setminus B(x,\varepsilon)} \frac{x-y}{|x-y|^n}\odot\nu(y)\,d\sigma(y) - \int_{\Omega\cap\partial B(x,\varepsilon)} \frac{x-y}{|x-y|^n}\odot\nu(y)\,d\mathcal{H}^{n-1}(y).
\end{aligned}\tag{5-13}$$

With this in hand, the first equality in (5-7) readily follows. Thus, (5-7) is fully proved.

To proceed, assume that $\Omega\subseteq\mathbb{R}^n$ is a bounded Lebesgue measurable set whose boundary is upper Ahlfors regular. Then (5-7) implies that, for each $x\in\mathbb{R}^n$,

$$\Big|\int_{\partial_*\Omega\setminus B(x,\varepsilon)} \frac{x-y}{|x-y|^n}\odot\nu(y)\,d\sigma(y)\Big| \le \frac{\mathcal{H}^{n-1}(\partial B(x,\varepsilon))}{\varepsilon^{n-1}} = \omega_{n-1}\tag{5-14}$$

for $\mathscr{L}^1$-a.e. $\varepsilon>0$. Now fix $x\in\mathbb{R}^n$ and pick an arbitrary $r\in(0,\infty)$. Based on (5-14) we conclude that there exists $\varepsilon\in\big(\tfrac{1}{2}r,r\big)$ such that

$$\Big|\int_{\partial_*\Omega\setminus B(x,\,\varepsilon)} \frac{x-y}{|x-y|^n}\odot\nu(y)\,d\sigma(y)\Big| \le \omega_{n-1}.\tag{5-15}$$

For this choice of ε we may then estimate

$$\begin{aligned}
&\Big|\int_{\partial_*\Omega\setminus B(x,r)} \frac{x-y}{|x-y|^n}\odot\nu(y)\,d\sigma(y)\Big|\\
&\qquad\le \Big|\int_{\partial_*\Omega\setminus B(x,\varepsilon)} \frac{x-y}{|x-y|^n}\odot\nu(y)\,d\sigma(y)\Big| + \Big|\int_{[B(x,r)\setminus B(x,\varepsilon)]\cap\partial_*\Omega} \frac{x-y}{|x-y|^n}\odot\nu(y)\,d\sigma(y)\Big|\\
&\qquad\le \omega_{n-1} + \int_{[B(x,r)\setminus B(x,\varepsilon)]\cap\partial\Omega} \frac{d\mathcal{H}^{n-1}(y)}{|x-y|^{n-1}}\\
&\qquad\le \omega_{n-1} + \int_{[B(x,2\varepsilon)\setminus B(x,\varepsilon)]\cap\partial\Omega} \frac{d\mathcal{H}^{n-1}(y)}{|x-y|^{n-1}}\\
&\qquad\le \omega_{n-1} + \varepsilon^{-(n-1)}\mathcal{H}^{n-1}(B(x,2\varepsilon)\cap\partial\Omega).
\end{aligned}\tag{5-16}$$

If $\operatorname{dist}(x, \partial\Omega) \le 2\varepsilon$, pick a point $x_0 \in \partial\Omega$ such that $\operatorname{dist}(x, \partial\Omega) = |x - x_0|$. In particular, $|x - x_0| \le 2\varepsilon$, which forces $B(x, 2\varepsilon) \subseteq B(x_0, 4\varepsilon)$. As such,

$$\mathcal{H}^{n-1}(B(x, 2\varepsilon) \cap \partial\Omega) \le \mathcal{H}^{n-1}(B(x_0, 4\varepsilon) \cap \partial\Omega) \le c(4\varepsilon)^{n-1}, \tag{5-17}$$

with $c \in (0, \infty)$ standing for the upper Ahlfors regularity constant of $\partial\Omega$. On the other hand, if $\operatorname{dist}(x, \partial\Omega) > 2\varepsilon$ then $\mathcal{H}^{n-1}(B(x, 2\varepsilon) \cap \partial\Omega) = 0$. Thus, taking $N := \omega_{n-1} + c\, 4^{n-1}$, the desired conclusion follows from (5-16) and (5-17) in the case when Ω is as in the statement of the lemma and also bounded.

Finally, when Ω is as in the statement of the lemma but unbounded, consider $\Omega^c := \mathbb{R}^n \setminus \Omega$. Then $\Omega^c \subseteq \mathbb{R}^n$ is a bounded, Lebesgue measurable set, with the property that $\partial(\Omega^c) = \partial\Omega$ and $\partial_*(\Omega^c) = \partial_*\Omega$. Moreover, the geometric measure-theoretic outward unit normal to Ω^c is $-\nu$. Then (5-6) follows from what we have proved so far applied to Ω^c. □

It is clear from (5-1) that the boundary-to-domain Cauchy–Clifford operator is well-defined on $L^1(\partial\Omega, \sigma)$. To state our next lemma, recall that $\rho(\cdot)$ has been introduced in (2-56).

Lemma 5.3. *Let Ω be a nonempty, proper, open subset of $\mathbb{R}^n$ whose boundary is compact, upper Ahlfors regular, and satisfies* (2-16). *Then the Cauchy–Clifford operator* (5-1) *has the property that, in Ω,*

$$\mathcal{C}1 = \begin{cases} 1 & \text{if } \Omega \text{ is bounded,} \\ 0 & \text{if } \Omega \text{ is unbounded,} \end{cases} \tag{5-18}$$

and for each $\alpha \in (0, 1)$ there exists a finite $M > 0$, depending only on n, α, $\operatorname{diam}(\partial\Omega)$, *and the upper Ahlfors regularity constant of $\partial\Omega$, such that for every $f \in \mathscr{C}^\alpha(\partial\Omega) \otimes \mathcal{C}\ell_n$ one has*

$$\sup_{x\in\Omega} |(\mathcal{C}f)(x)| + \sup_{x\in\Omega}\bigl\{\rho(x)^{1-\alpha} |\nabla(\mathcal{C}f)(x)|\bigr\} \le M \|f\|_{\mathscr{C}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n}. \tag{5-19}$$

Proof. The fact that $\mathcal{C}1 = 1$ in Ω when Ω is bounded follows from (5-7), written for $x \in \Omega$ and suitably small $\varepsilon > 0$. That $(\mathcal{C}1)(x) = 0$ for each $x \in \Omega$ when Ω is unbounded also follows from (5-7), this time considered for the bounded set $\Omega^c := \mathbb{R}^n \setminus \Omega$ (since in this case $\Omega^c \cap \partial B(x, \varepsilon) = \varnothing$ if $\varepsilon > 0$ is sufficiently small). Having proved (5-18), the inequality (5-19) follows with the help of Lemma 3.5. □

In contrast to Lemma 5.3 (see also Lemma 5.4 below), we note that there exists a bounded open set $\Omega \subset \mathbb{R}^2 \equiv \mathbb{C}$ whose boundary is a rectifiable Jordan curve, and there exists a complex-valued function $f \in \mathscr{C}^{1/2}(\partial\Omega)$ with the property that the boundary-to-domain Cauchy operator naturally associated with Ω acting on f is actually an unbounded function in Ω. See the discussion in [Dyn′kin 1979; 1980].

Lemma 5.4. *Let $\Omega \subset \mathbb{R}^n$ be a uniform domain whose boundary is compact, upper Ahlfors regular, and satisfies* (2-16). *Then the boundary-to-domain Cauchy–Clifford operator, for each $\alpha \in (0, 1)$, is well-defined, linear and bounded in the context*

$$\mathcal{C} : \mathscr{C}^\alpha(\partial\Omega) \otimes \mathcal{C}\ell_n \longrightarrow \mathscr{C}^\alpha(\overline{\Omega}) \otimes \mathcal{C}\ell_n, \tag{5-20}$$

with operator norm controlled in terms of n, α, $\operatorname{diam}(\partial\Omega)$, *and the upper Ahlfors regularity constant of $\partial\Omega$.*

Proof. This is a direct consequence of Lemmas 5.3 and 2.10. □

In the class of UR domains with compact boundaries that are also uniform domains, it follows from Lemma 5.4 and the jump formula (5-3) that the principal value Cauchy–Clifford operator $\mathcal{C}^{\mathrm{pv}}$ defines a bounded mapping from $\mathscr{C}^{\alpha}(\partial\Omega) \otimes \mathcal{C}\ell_n$ into itself for each $\alpha \in (0, 1)$. The goal is to prove that this boundedness result actually holds under much more relaxed background assumptions on the underlying domain. In this regard, a key aspect has to do with the action of $\mathcal{C}^{\mathrm{pv}}$ on constants. Note that when $\Omega \subset \mathbb{R}^n$ is a UR domain with compact boundary, it follows from (5-18) and (5-3) that the principal value Cauchy–Clifford operator satisfies, on $\partial\Omega$,

$$\mathcal{C}^{\mathrm{pv}}1 = \begin{cases} +\frac{1}{2} & \text{if } \Omega \text{ is bounded,} \\ -\frac{1}{2} & \text{if } \Omega \text{ is unbounded.} \end{cases} \tag{5-21}$$

The lemma below establishes a formula similar in spirit to (5-21) but for a much larger class of sets $\Omega \subset \mathbb{R}^n$ than the category of UR domains with compact boundaries.

Lemma 5.5. *Let $\Omega \subset \mathbb{R}^n$ be a Lebesgue measurable set whose boundary is compact, Ahlfors regular, and such that* (2-16) *is satisfied* (*hence, in particular, Ω has locally finite perimeter*). *As in the past, consider $\sigma := \mathcal{H}^{n-1}\lfloor\partial\Omega$ and let ν denote the outward unit normal to Ω. Then for σ-a.e. $x \in \partial\Omega$ there holds*

$$\lim_{\varepsilon\to 0^+} \frac{1}{\omega_{n-1}} \int_{\substack{y\in\partial\Omega \\ |x-y|>\varepsilon}} \frac{x-y}{|x-y|^n} \odot \nu(y)\, d\sigma(y) = \begin{cases} +\frac{1}{2} & \text{if } \Omega \text{ is bounded,} \\ -\frac{1}{2} & \text{if } \Omega \text{ is unbounded.} \end{cases} \tag{5-22}$$

Proof. Consider first the case when Ω is bounded. Fix $x \in \partial^*\Omega$ and pick an arbitrary $\delta > 0$. From Lemma 2.5 we know that there exist $\mathcal{O}_x \subset (0, 1)$ of density 1 at 0 (i.e., satisfying (2-33)) and some $r_\delta > 0$ with the property that

$$\left| \frac{\mathcal{H}^{n-1}(\Omega \cap \partial B(x, r))}{\omega_{n-1} r^{n-1}} - \frac{1}{2} \right| < \delta \quad \text{for all } r \in \mathcal{O}_x \cap (0, r_\delta). \tag{5-23}$$

Since (2-33) entails

$$\lim_{\varepsilon\to 0^+} \frac{\mathscr{L}^1\big(\mathcal{O}_x \cap \big(\frac{1}{2}\varepsilon, \varepsilon\big)\big)}{\varepsilon} = \lim_{\varepsilon\to 0^+} \frac{\mathscr{L}^1(\mathcal{O}_x \cap (0, \varepsilon))}{\varepsilon} - \lim_{\varepsilon\to 0^+} \frac{\mathscr{L}^1\big(\mathcal{O}_x \cap \big(0, \frac{1}{2}\varepsilon\big)\big)}{\varepsilon} = 1 - \tfrac{1}{2} = \tfrac{1}{2}, \tag{5-24}$$

it follows that there exists $\varepsilon_\delta \in (0, r_\delta)$ with the property that

$$\mathscr{L}^1\big(\mathcal{O}_x \cap \big(\tfrac{1}{2}\varepsilon, \varepsilon\big)\big) > 0 \quad \text{for all } \varepsilon \in (0, \varepsilon_\delta). \tag{5-25}$$

From our assumptions on Ω and (5-7) we also know that there exists $N_x \subset (0, \infty)$ with $\mathscr{L}^1(N_x) = 0$ such that for all $r \in (0, \infty) \setminus N_x$ we have

$$\frac{1}{\omega_{n-1}} \int_{\substack{y\in\partial\Omega \\ |x-y|>r}} \frac{x-y}{|x-y|^n} \odot \nu(y)\, d\sigma(y) = \frac{\mathcal{H}^{n-1}(\Omega \cap \partial B(x, r))}{\omega_{n-1} r^{n-1}}. \tag{5-26}$$

Consider next $\varepsilon \in (0, \varepsilon_\delta)$ and note that $\big[\mathcal{O}_x \cap \big(\tfrac{1}{2}\varepsilon, \varepsilon\big)\big] \setminus N_x \neq \varnothing$, thanks to (5-25). As such, it is possible to select $r \in \big[\mathcal{O}_x \cap \big(\tfrac{1}{2}\varepsilon, \varepsilon\big)\big] \setminus N_x$, for which we then write

$$\begin{aligned}\int_{\substack{y\in\partial\Omega\\|x-y|>\varepsilon/4}} &\frac{x-y}{|x-y|^n} \odot \nu(y)\, d\sigma(y)\\ &= \int_{\substack{y\in\partial\Omega\\ r\geq|x-y|>\varepsilon/4}} \frac{x-y}{|x-y|^n} \odot \nu(y)\, d\sigma(y) + \int_{\substack{y\in\partial\Omega\\|x-y|>r}} \frac{x-y}{|x-y|^n} \odot \nu(y)\, d\sigma(y).\end{aligned} \tag{5-27}$$

In turn, (5-27), (5-26) and (5-23) permit us to estimate

$$\begin{aligned}\bigg|\frac{1}{\omega_{n-1}} \int_{\substack{y\in\partial\Omega\\|x-y|>\varepsilon/4}} &\frac{x-y}{|x-y|^n} \odot \nu(y)\, d\sigma(y) - \frac{1}{2}\bigg|\\ &\leq \bigg|\frac{1}{\omega_{n-1}} \int_{\substack{y\in\partial\Omega\\ r\geq|x-y|>\varepsilon/4}} \frac{x-y}{|x-y|^n} \odot \nu(y)\, d\sigma(y)\bigg| + \bigg|\frac{\mathcal{H}^{n-1}(\Omega\cap\partial B(x,r))}{\omega_{n-1}r^{n-1}} - \frac{1}{2}\bigg|\\ &\leq \sup_{r\in(\varepsilon/2,\varepsilon)} \bigg|\frac{1}{\omega_{n-1}} \int_{\substack{y\in\partial\Omega\\ r\geq|x-y|>\varepsilon/4}} \frac{x-y}{|x-y|^n} \odot \nu(y)\, d\sigma(y)\bigg| + \delta,\end{aligned} \tag{5-28}$$

which, in light of Proposition 2.4 (whose applicability in the current setting is ensured by (2-19)), then yields (bearing in mind (2-14))

$$\limsup_{\varepsilon\to 0^+} \bigg|\frac{1}{\omega_{n-1}} \int_{\substack{y\in\partial\Omega\\|x-y|>\varepsilon/4}} \frac{x-y}{|x-y|^n} \odot \nu(y)\, d\sigma(y) - \frac{1}{2}\bigg| \leq \delta \quad \text{for } \sigma\text{-a.e. } x \in \partial\Omega. \tag{5-29}$$

Given that $\delta > 0$ has been arbitrarily chosen, the version of (5-22) for Ω bounded readily follows from this. Finally, the version of (5-22) corresponding to Ω unbounded is a consequence of what we have proved so far, applied to the bounded set $\Omega^c := \mathbb{R}^n \setminus \Omega$ (whose geometric measure-theoretic outward unit normal is $-\nu$). □

The stage has been set to show that, under much less restrictive conditions on the underlying set Ω (than the class of UR domains with compact boundaries that are also uniform domains), the principal value Cauchy–Clifford operator $\mathcal{C}^{\mathrm{pv}}$ continues to be a bounded mapping from $\mathscr{C}^\alpha(\partial\Omega) \otimes \mathcal{C}\ell_n$ into itself for each $\alpha \in (0, 1)$. In this regard, our result can be thought of as the higher-dimensional generalization of the classical Plemelj–Privalov theorem, according to which the Cauchy integral operator on a piecewise smooth Jordan curve without cusps in the plane is bounded on Hölder spaces (see [Plemelj 1908; Privalov 1918; 1941], as well as the discussion in [Muskhelishvili 1953, §19, pp. 45–49]). In addition, we also establish a natural jump formula and prove that $2\mathcal{C}^{\mathrm{pv}}$ is idempotent on $\mathscr{C}^\alpha(\partial\Omega) \otimes \mathcal{C}\ell_n$ for $\alpha \in (0, 1)$. We wish to stress that, even in the more general geometric measure-theoretic setting considered below, we retain (5-2) as the definition of the Cauchy–Clifford operator $\mathcal{C}^{\mathrm{pv}}$.

Theorem 5.6. *Let $\Omega \subset \mathbb{R}^n$ be a Lebesgue measurable set whose boundary is compact, upper Ahlfors regular, and satisfies* (2-16). *As in the past, define $\sigma := \mathcal{H}^{n-1}\lfloor\partial\Omega$, and fix an arbitrary $\alpha \in (0, 1)$.*

Then for each $f \in \mathscr{C}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n$ *the limit defining* $\mathcal{C}^{\mathrm{pv}} f(x)$ *as in* (5-2) *exists for* σ*-a.e.* $x \in \partial\Omega$, *and the operator* $\mathcal{C}^{\mathrm{pv}}$ *induces a well-defined, linear and bounded mapping*

$$\mathcal{C}^{\mathrm{pv}} : \mathscr{C}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n \longrightarrow \mathscr{C}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n. \tag{5-30}$$

Furthermore, under the additional assumption that the set Ω *is open, the jump formula*

$$(\mathcal{C}f)\big|^{\mathrm{nt}}_{\partial\Omega} = \big(\tfrac{1}{2}I + \mathcal{C}^{\mathrm{pv}}\big)f \quad \textit{at } \sigma\textit{-a.e. point in } \partial\Omega \tag{5-31}$$

is valid for every function $f \in \mathscr{C}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n$, *and one also has*

$$(\mathcal{C}^{\mathrm{pv}})^2 = \tfrac{1}{4}I \quad \textit{on } \mathscr{C}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n. \tag{5-32}$$

Incidentally, given an open set Ω in the plane, the fact that its boundary is a piecewise smooth Jordan curve implies that $\partial\Omega$ is compact and upper Ahlfors regular, while the additional property that $\partial\Omega$ lacks cusps implies that (2-16) holds. Hence, our demands on the underlying domain Ω are weaker versions of the hypotheses in the formulation of the classical Plemelj–Privalov theorem mentioned earlier.

Proof of Theorem 5.6. Fix $\alpha \in (0,1)$ and pick an arbitrary function $f \in \mathscr{C}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n$. Then, for σ-a.e. $x \in \partial\Omega$, Lemma 5.5 allows us to write

$$\begin{aligned}
&\lim_{\varepsilon\to 0^+} \frac{1}{\omega_{n-1}} \int_{\substack{y\in\partial\Omega\\ |x-y|>\varepsilon}} \frac{x-y}{|x-y|^n} \odot \nu(y) \odot f(y)\, d\sigma(y) \\
&\qquad = \lim_{\varepsilon\to 0^+} \frac{1}{\omega_{n-1}} \int_{\substack{y\in\partial\Omega\\ |x-y|>\varepsilon}} \frac{x-y}{|x-y|^n} \odot \nu(y) \odot (f(y)-f(x))\, d\sigma(y) \pm \tfrac{1}{2} f(x) \\
&\qquad = \frac{1}{\omega_{n-1}} \int_{\partial\Omega} \frac{x-y}{|x-y|^n} \odot \nu(y) \odot (f(y)-f(x))\, d\sigma(y) \pm \tfrac{1}{2} f(x),
\end{aligned} \tag{5-33}$$

where the sign of $\frac{1}{2}f(x)$ is plus if Ω is bounded and minus if Ω is unbounded. For the last equality, we have used Lebesgue's dominated convergence theorem. Indeed, given that $f(y)-f(x) = O(|x-y|^\alpha)$, an estimate based on the upper Ahlfors regularity of $\partial\Omega$ in the spirit of (3-39) shows that the last integrand above is absolutely integrable for each fixed $x \in \partial\Omega$. In turn, (5-33) allows us to conclude that the limit defining $\mathcal{C}^{\mathrm{pv}} f(x)$ in (5-2) exists for σ-a.e. $x \in \partial\Omega$. Furthermore, by redefining $\mathcal{C}^{\mathrm{pv}} f$ on a set of zero σ-measure, there is no loss of generality in assuming that, for each $f \in \mathscr{C}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n$ with $\alpha \in (0,1)$,

$$\mathcal{C}^{\mathrm{pv}} f(x) = \pm\tfrac{1}{2} f(x) + \frac{1}{\omega_{n-1}} \int_{\partial\Omega} \frac{x-y}{|x-y|^n} \odot \nu(y) \odot (f(y)-f(x))\, d\sigma(y) \quad \text{for all } x \in \partial\Omega, \tag{5-34}$$

with the sign dictated by whether Ω is bounded (plus) or unbounded (minus).

We now proceed to showing that, in the context of (5-30), the operator (5-34) is well-defined and bounded. To this end, fix distinct points $x_1, x_2 \in \partial\Omega$ and, starting from (5-34), write

$$\mathcal{C}^{\mathrm{pv}} f(x_1) - \mathcal{C}^{\mathrm{pv}} f(x_2) = I + II, \tag{5-35}$$

where

$$I := \pm\tfrac{1}{2}(f(x_1) - f(x_2)) \tag{5-36}$$

and

$$II := \frac{1}{\omega_{n-1}} \int_{\partial\Omega} \left\{ \frac{x_1 - y}{|x_1 - y|^n} \odot \nu(y) \odot (f(y) - f(x_1)) - \frac{x_2 - y}{|x_2 - y|^n} \odot \nu(y) \odot (f(y) - f(x_2)) \right\} d\sigma(y). \tag{5-37}$$

Next, introduce $r := |x_1 - x_2| > 0$ and estimate

$$|II| \leq II_1 + II_2 + II_3, \tag{5-38}$$

where

$$II_1 := \frac{1}{\omega_{n-1}} \left| \int_{\substack{y \in \partial\Omega \\ |x_1 - y| > 2r}} \frac{x_1 - y}{|x_1 - y|^n} \odot \nu(y) \odot (f(y) - f(x_1)) - \frac{x_2 - y}{|x_2 - y|^n} \odot \nu(y) \odot (f(y) - f(x_2))\, d\sigma(y) \right|, \tag{5-39}$$

while

$$II_2 := \frac{1}{\omega_{n-1}} \int_{\substack{y \in \partial\Omega \\ |x_1 - y| \leq 2r}} \left| \frac{x_1 - y}{|x_1 - y|^n} \odot \nu(y) \odot (f(y) - f(x_1)) \right| d\sigma(y), \tag{5-40}$$

$$II_3 := \frac{1}{\omega_{n-1}} \int_{\substack{y \in \partial\Omega \\ |x_1 - y| \leq 2r}} \left| \frac{x_2 - y}{|x_2 - y|^n} \odot \nu(y) \odot (f(y) - f(x_2)) \right| d\sigma(y). \tag{5-41}$$

Note that

$$II_2 \leq c_n [f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega) \otimes \mathcal{C}\ell_n} \int_{\substack{y \in \partial\Omega \\ |x_1 - y| \leq 2r}} \frac{d\sigma(y)}{|x_1 - y|^{n-1-\alpha}}, \tag{5-42}$$

and, given that $|x_1 - y| \leq 2r$ forces $|x_2 - y| \leq |x_1 - x_2| + |x_1 - y| \leq 3r$,

$$\begin{aligned} II_3 &\leq \frac{1}{\omega_{n-1}} \int_{\substack{y \in \partial\Omega \\ |x_2 - y| \leq 3r}} \left| \frac{x_2 - y}{|x_2 - y|^n} \odot \nu(y) \odot (f(y) - f(x_2)) \right| d\sigma(y) \\ &\leq c_n [f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega) \otimes \mathcal{C}\ell_n} \int_{\substack{y \in \partial\Omega \\ |x_2 - y| \leq 3r}} \frac{d\sigma(y)}{|x_2 - y|^{n-1-\alpha}}. \end{aligned} \tag{5-43}$$

On the other hand, with $c \in (0, \infty)$ denoting the upper Ahlfors regularity constant of $\partial\Omega$, for every $z \in \partial\Omega$ and $R \in (0, \infty)$ we may estimate

$$\begin{aligned} \int_{\substack{y \in \partial\Omega \\ |z - y| < R}} \frac{d\sigma(y)}{|z - y|^{n-1-\alpha}} &= \sum_{j=1}^{\infty} \int_{[B(z, 2^{1-j}R) \setminus B(z, 2^{-j}R)] \cap \partial\Omega} \frac{d\sigma(y)}{|z - y|^{n-1-\alpha}} \\ &\leq \sum_{j=1}^{\infty} (2^{-j}R)^{-(n-1-\alpha)} \sigma(B(z, 2^{1-j}R) \cap \partial\Omega) \\ &\leq c 2^{n-1} \sum_{j=1}^{\infty} (2^{-j}R)^\alpha = M R^\alpha \end{aligned} \tag{5-44}$$

for some constant $M = M(n, \alpha, c) \in (0, \infty)$. In light of this, we obtain from (5-42) and (5-43) (keeping in mind the significance of the number r) that there exists some constant $M = M(n, \alpha, c) \in (0, \infty)$ with the property that

$$II_2 + II_3 \le M[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)}|x_1 - x_2|^\alpha. \tag{5-45}$$

Going further, bound

$$II_1 \le II_1^a + II_1^b, \tag{5-46}$$

where

$$\begin{aligned} II_1^a &:= \frac{1}{\omega_{n-1}}\left|\int_{\substack{y\in\partial\Omega\\|x_1-y|>2r}} \frac{x_1-y}{|x_1-y|^n}\odot\nu(y)\odot(f(x_2)-f(x_1))\,d\sigma(y)\right| \\ &= \frac{1}{\omega_{n-1}}\left|\left(\int_{\substack{y\in\partial\Omega\\|x_1-y|>2r}} \frac{x_1-y}{|x_1-y|^n}\odot\nu(y)\,d\sigma(y)\right)\odot(f(x_2)-f(x_1))\right| \\ &\le \frac{2^{n/2}}{\omega_{n-1}}\left|\int_{\substack{y\in\partial\Omega\\|x_1-y|>2r}} \frac{x_1-y}{|x_1-y|^n}\odot\nu(y)\,d\sigma(y)\right||f(x_2)-f(x_1)| \\ &\le M(n,c)r^\alpha[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n}, \end{aligned} \tag{5-47}$$

where the penultimate inequality uses (4-13) while the last inequality is based on (5-6), and

$$\begin{aligned} II_1^b &:= \frac{1}{\omega_{n-1}}\left|\int_{\substack{y\in\partial\Omega\\|x_1-y|>2r}} \left(\frac{x_1-y}{|x_1-y|^n}-\frac{x_2-y}{|x_2-y|^n}\right)\odot\nu(y)\odot(f(y)-f(x_2))\,d\sigma(y)\right| \\ &\le \frac{2^{n/2}}{\omega_{n-1}}\int_{\substack{y\in\partial\Omega\\|x_1-y|>2r}} \left|\frac{x_1-y}{|x_1-y|^n}-\frac{x_2-y}{|x_2-y|^n}\right||f(y)-f(x_2)|\,d\sigma(y) \\ &\le c_n r[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n}\int_{\substack{y\in\partial\Omega\\|x_1-y|>2r}} \frac{d\sigma(y)}{|x_1-y|^{n-\alpha}}, \end{aligned} \tag{5-48}$$

using the mean value theorem and the fact that f is Hölder of order α. Here it helps to note that if $y \in \partial\Omega$ and $|x_1 - y| > 2r$ then $|\xi - y| \approx |x_1 - y|$ for all $\xi \in [x_1, x_2]$, and also $|y - x_2| < \frac{1}{2}|y - x_1|$. To continue, with $c \in (0, \infty)$ denoting the upper Ahlfors regularity constant of $\partial\Omega$ we observe that

$$\begin{aligned} \int_{\substack{y\in\partial\Omega\\|x_1-y|>2r}} \frac{d\sigma(y)}{|x_1-y|^{n-\alpha}} &= \sum_{j=1}^{\infty}\int_{[B(x_1,2^{j+1}r)\setminus B(x_1,2^j r)]\cap\partial\Omega} \frac{d\sigma(y)}{|x_1-y|^{n-\alpha}} \\ &\le \sum_{j=1}^{\infty}(2^j r)^{-(n-\alpha)}\sigma(B(x_1,2^{j+1}r)\cap\partial\Omega) \\ &\le c^{n-1}\sum_{j=1}^{\infty}(2^j r)^{-1+\alpha} = Mr^{-1+\alpha} \end{aligned} \tag{5-49}$$

for some constant $M = M(n, \alpha, c) \in (0, \infty)$. Combining (5-46)–(5-49) we conclude that there exists a constant $M = M(n, \alpha, c) \in (0, \infty)$ with the property that

$$II_1 \le M[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n}|x_1 - x_2|^\alpha. \tag{5-50}$$

From (5-35)–(5-36), (5-38), (5-45) and (5-50) we may then conclude that

$$|\mathcal{C}^{\mathrm{pv}} f(x_1) - \mathcal{C}^{\mathrm{pv}} f(x_2)| \leq M[f]_{\dot{\mathscr{C}}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n} |x_1 - x_2|^\alpha \quad \text{for all } x_1, x_2 \in \partial\Omega \tag{5-51}$$

for some constant $M = M(n, \alpha, c) \in (0, \infty)$. The argument so far gives that the Cauchy–Clifford singular integral operator $\mathcal{C}^{\mathrm{pv}}$ maps $\dot{\mathscr{C}}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n$ boundedly into itself. Having established this, Lemma 3.3 may be invoked — bearing in mind that (5-34) forces $\mathcal{C}^{\mathrm{pv}} 1 = \pm\frac{1}{2}$ — in order to finish the proof of the theorem.

Turning our attention to the last part of the statement of the theorem, make the additional assumption that the set Ω is open. As far as the jump formula (5-31) is concerned, it has been already noted that the action of the boundary-to-domain Cauchy–Clifford operator (5-1) is meaningful on Hölder functions. Also, Proposition 2.8 ensures that it is meaningful to consider the nontangential boundary trace in the left-hand side of (5-31) given that $\Omega \subseteq \mathbb{R}^n$ is an open set with an Ahlfors regular boundary satisfying (2-16) (hence, Ω is an Ahlfors regular domain; see Definition 2.3). Assume now that some $f \in \mathscr{C}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n$ with $\alpha \in (0, 1)$ has been given and observe that $\mathcal{C} f$ is continuous in Ω. Fix $x \in \partial^*\Omega$ and let $\mathcal{O}_x$ be the set given by Lemma 2.5 applied with Ω replaced by the Lebesgue measurable set $\mathbb{R}^n \setminus \Omega$. In particular,

$$\lim_{\substack{\varepsilon\to 0^+\\ \varepsilon\in\mathcal{O}_x}} \frac{\mathcal{H}^{n-1}(\partial B(x,\varepsilon)\setminus\Omega)}{\omega_{n-1}\varepsilon^{n-1}} = \frac{1}{2}. \tag{5-52}$$

For some $\kappa > 0$ fixed, write

$$\begin{aligned}
\lim_{\substack{z\to x\\ z\in\Gamma_\kappa(x)}} \mathcal{C} f(z) &= \lim_{\substack{\varepsilon\to 0^+\\ \varepsilon\in\mathcal{O}_x}} \lim_{\substack{z\to x\\ z\in\Gamma_\kappa(x)}} \frac{1}{\omega_{n-1}} \int_{\substack{|x-y|>\varepsilon\\ y\in\partial\Omega}} \frac{z-y}{|z-y|^n} \odot \nu(y) \odot f(y)\, d\sigma(y) \\
&\qquad + \lim_{\substack{\varepsilon\to 0^+\\ \varepsilon\in\mathcal{O}_x}} \lim_{\substack{z\to x\\ z\in\Gamma_\kappa(x)}} \frac{1}{\omega_{n-1}} \int_{\substack{|x-y|<\varepsilon\\ y\in\partial\Omega}} \frac{z-y}{|z-y|^n} \odot \nu(y) \odot (f(y) - f(x))\, d\sigma(y) \\
&\qquad\quad + \Bigg(\lim_{\substack{\varepsilon\to 0^+\\ \varepsilon\in\mathcal{O}_x}} \lim_{\substack{z\to x\\ z\in\Gamma_\kappa(x)}} \frac{1}{\omega_{n-1}} \int_{\substack{|x-y|<\varepsilon\\ y\in\partial\Omega}} \frac{z-y}{|z-y|^n} \odot \nu(y)\, d\sigma(y) \Bigg) \odot f(x) \\
&=: I_1 + I_2 + I_3.
\end{aligned} \tag{5-53}$$

For each fixed $\varepsilon > 0$, Lebesgue's dominated convergence theorem applies to the limit as $z \to x$, $z \in \Gamma_\kappa(x)$, in I_1 and yields

$$I_1 = \lim_{\varepsilon\to 0^+} \frac{1}{\omega_{n-1}} \int_{\substack{|x-y|>\varepsilon\\ y\in\partial\Omega}} \frac{x-y}{|x-y|^n} \odot \nu(y) \odot f(y)\, d\sigma(y) = \mathcal{C}^{\mathrm{pv}} f(x). \tag{5-54}$$

To handle I_2, we first observe that, for every $x, y \in \partial\Omega$ and $z \in \Gamma_\kappa(x)$,

$$|x-y| \leq |z-y| + |z-x| \leq |z-y| + (1+\kappa)\operatorname{dist}(z, \partial\Omega) \leq |z-y| + (1+\kappa)|z-y| = (2+\kappa)|z-y|. \tag{5-55}$$

Hence, since f is Hölder of order α,

$$\left| \frac{z-y}{|z-y|^n} \odot \nu(y) \right| |f(y) - f(x)| \leq [f]_{\mathscr{C}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n} \frac{(2+\kappa)^{n-1}}{|x-y|^{n-1-\alpha}}, \tag{5-56}$$

so that, based on the upper Ahlfors regularity of $\partial\Omega$ and once again Lebesgue's dominated convergence theorem, we obtain that

$$I_2 = 0. \tag{5-57}$$

To treat I_3 in (5-53), we first claim that, having fixed $z \in \Omega$, for $\mathscr{L}^1$-a.e $\varepsilon > 0$ we have

$$\int_{\substack{|x-y|<\varepsilon \\ y\in\partial\Omega}} \frac{z-y}{|z-y|^n} \odot \nu(y)\, d\sigma(y) = \int_{\substack{|x-y|=\varepsilon \\ y\in\mathbb{R}^n\setminus\Omega}} \frac{z-y}{|z-y|^n} \odot \nu(y)\, d\sigma(y). \tag{5-58}$$

To justify this, pick a large $R > 0$ and apply (2-61) to $D := B(0, R) \setminus \Omega$ and, for each $j, k \in \{1, \dots, n\}$, to the vector field

$$\vec{F}_{jk}(y) := \left(0, \dots, 0, \frac{z_j - y_j}{|z-y|^n}, 0, \dots, 0\right) \quad \text{for all } y \in \mathbb{R}^n \setminus \{z\}, \tag{5-59}$$

with the nonzero component in the k-th slot. We can alter each $\vec{F}_{jk}$ outside a compact neighborhood of $\overline{D}$ to a vector field $\vec{G}_{jk} \in \mathscr{C}^1_0(\mathbb{R}^n \setminus \{z\}, \mathbb{R}^n)$. Then (5-58) follows by reasoning as in (5-11)–(5-13). Consequently, starting with (5-58), then using (5-8), and then (5-52), we obtain

$$\begin{aligned}\lim_{\substack{\varepsilon\to 0^+ \\ \varepsilon\in\mathcal{O}_x}} \lim_{\substack{z\to x \\ z\in\Gamma_\kappa(x)}} \frac{1}{\omega_{n-1}} \int_{\substack{|x-y|<\varepsilon \\ y\in\partial\Omega}} \frac{z-y}{|z-y|^n} \odot \nu(y)\, d\sigma(y) &= \lim_{\substack{\varepsilon\to 0^+ \\ \varepsilon\in\mathcal{O}_x}} \frac{1}{\omega_{n-1}} \int_{\substack{|x-y|=\varepsilon \\ y\in\mathbb{R}^n\setminus\Omega}} \frac{x-y}{|x-y|^n} \odot \nu(y)\, d\sigma(y) \\ &= \lim_{\substack{\varepsilon\to 0^+ \\ \varepsilon\in\mathcal{O}_x}} \frac{\mathcal{H}^{n-1}(\partial B(x,\varepsilon)\setminus\Omega)}{\omega_{n-1}\varepsilon^{n-1}} = \frac{1}{2}.\end{aligned} \tag{5-60}$$

A combination of (5-53), (5-54), (5-57) and (5-60) shows that the limit in the left-hand side of (5-53) exists and matches $\left(\frac{1}{2}I + \mathcal{C}^{\mathrm{pv}}\right) f(x)$. This proves that (5-31) holds for each $f \in \mathscr{C}^\alpha(\partial\Omega) \otimes \mathcal{C}\ell_n$ at every $x \in \partial^*\Omega$, hence at σ-a.e. point in $\partial\Omega$, by (2-14) and the assumption (2-16).

To finish the proof of the theorem, it remains to establish (5-32) assuming, again, that the set Ω is open. Suppose this is the case and introduce the version of the Cauchy reproducing formula from [Mitrea et al. 2015, Section 3] to the effect that, under the current assumptions on the set Ω,

$$\begin{aligned}&u : \Omega \to \mathcal{C}\ell_n \text{ continuous, with } D_L u = 0 \text{ in } \Omega,\ \mathcal{N}u \in L^1(\partial\Omega, \sigma) \text{ and } u\big|^{\mathrm{nt}}_{\partial\Omega} \text{ exists } \sigma\text{-a.e. on } \partial\Omega \\ &\qquad\qquad \Longrightarrow\ u = \mathcal{C}(u\big|^{\mathrm{nt}}_{\partial\Omega}) \text{ in } \Omega.\end{aligned} \tag{5-61}$$

Now, given any $f \in \mathscr{C}^\alpha(\partial\Omega) \otimes \mathcal{C}\ell_n$, define $u := \mathcal{C} f$ in Ω. Then, by design, $u \in \mathscr{C}^\infty(\Omega)$ and $D_L u = 0$ in Ω. Also, (5-19) gives that $\sup_{x\in\Omega} |u(x)| \le M\|f\|_{\mathscr{C}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n}$, which, in turn, forces $\mathcal{N}u$ to be in $L^\infty(\partial\Omega, \sigma) \subset L^1(\partial\Omega, \sigma)$, given that $\partial\Omega$ has finite measure. Finally, the jump formula (5-3) for Hölder functions, established earlier in the proof, yields

$$(u\big|^{\mathrm{nt}}_{\partial\Omega})(x) = \left(\tfrac{1}{2}I + \mathcal{C}^{\mathrm{pv}}\right) f(x) \quad \text{for } \sigma\text{-a.e. } x \in \partial\Omega. \tag{5-62}$$

Granted these, the premise of (5-61) holds and gives

$$u = \mathcal{C}(u\big|^{\mathrm{nt}}_{\partial\Omega}) \quad \text{in } \Omega. \tag{5-63}$$

Moreover, since $f \in \mathscr{C}^\alpha(\partial\Omega) \otimes \mathcal{C}\ell_n$ and $\mathcal{C}^{\text{pv}}$ is a well-defined mapping in the context of (5-30), from (5-62) we see that

$$u\big|_{\partial\Omega}^{\text{nt}} \in \mathscr{C}^\alpha(\partial\Omega) \otimes \mathcal{C}\ell_n. \tag{5-64}$$

Going to the boundary nontangentially in (5-63) and relying on (5-62) and (5-31) (bearing in mind (5-64)) then allows us to write

$$\big(\tfrac{1}{2}I + \mathcal{C}^{\text{pv}}\big)f = \big(\tfrac{1}{2}I + \mathcal{C}^{\text{pv}}\big)\big(\tfrac{1}{2}I + \mathcal{C}^{\text{pv}}\big)f \quad \text{at } \sigma\text{-a.e. point on } \partial\Omega, \tag{5-65}$$

from which (5-32) now readily follows. □

In the last part of this section we briefly consider harmonic layer potentials. Recall the standard fundamental solution E_Δ for the Laplacian in $\mathbb{R}^n$ from (5-10). Given a nonempty, open, proper subset Ω of $\mathbb{R}^n$, let $\sigma := \mathcal{H}^{n-1}\lfloor\partial\Omega$. Then the *harmonic single layer operator* associated with Ω acts on a function f defined on $\partial\Omega$ by

$$\mathscr{S}f(x) := \int_{\partial\Omega} E_\Delta(x-y) f(y)\, d\sigma(y), \quad x \in \Omega. \tag{5-66}$$

Assume that Ω is a set of locally finite perimeter for which (2-16) holds and denote by ν its (geometric measure-theoretic) outward unit normal. In this context, it follows from (4-17), (5-66), (5-1) and the fact that $\nu \odot \nu = -1$ (see (4-1)) that the harmonic single layer operator and the Cauchy–Clifford operator are related via

$$D_L \mathscr{S} f = -\mathcal{C}(\nu \odot f) \quad \text{in } \Omega. \tag{5-67}$$

Parenthetically, we wish to note that, in the same setting, the *harmonic double layer operator* associated with Ω is defined as

$$\mathscr{D}f(x) := \frac{1}{\omega_{n-1}} \int_{\partial\Omega} \frac{\langle \nu(y), y-x\rangle}{|x-y|^n} f(y)\, d\sigma(y), \quad x \in \Omega, \tag{5-68}$$

where $\langle\cdot,\cdot\rangle$ is the standard inner product of vectors in $\mathbb{R}^n$. In particular, from (5-1), (4-10), (4-8) and (5-68), it follows that

$$f \text{ scalar-valued} \quad \Longrightarrow \quad \mathscr{D}f = (\mathcal{C}f)_0 \text{ in } \Omega. \tag{5-69}$$

As a consequence of this and (5-20), we see that if $\Omega \subset \mathbb{R}^n$ is a uniform domain whose boundary is compact, upper Ahlfors regular, and satisfies (2-16) then, for each $\alpha \in (0, 1)$, the harmonic double layer operator induces a well-defined, linear and bounded mapping

$$\mathscr{D} : \mathscr{C}^\alpha(\partial\Omega) \longrightarrow \mathscr{C}^\alpha(\overline{\Omega}). \tag{5-70}$$

Returning to the main discussion, make the convention that ∇^2 is the vector of all second-order partial derivatives in $\mathbb{R}^n$. Also, once again, recall (2-56).

Lemma 5.7. *Let Ω be a domain of class $\mathscr{C}^{1+\alpha}$ for some $\alpha \in (0, 1)$ with compact boundary. Then*

$$A := \sup_{x\in\Omega} |\nabla(\mathscr{S}1)(x)| + \sup_{x\in\Omega}\big\{\rho(x)^{1-\alpha}|\nabla^2(\mathscr{S}1)(x)|\big\} < +\infty \tag{5-71}$$

and, in fact, this quantity may be estimated in terms of n, α, $\mathrm{diam}(\partial\Omega)$, $\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)}$ *and the upper Ahlfors regularity constant of* $\partial\Omega$.

Proof. Via the identification (4-3) we obtain from (5-67) that

$$\nabla(\mathscr{S}1) \equiv D_L\mathscr{S}1 = -\mathcal{C}\nu \quad \text{in } \Omega. \tag{5-72}$$

Then, keeping in mind that $\nu \in \mathscr{C}^\alpha(\partial\Omega)\otimes \mathcal{C}\ell_n$ under the present assumption on Ω, the claim in (5-71) readily follows by combining (5-72) with (5-19). □

6. The proofs of Theorems 1.1 and 1.3

We start by presenting the proof of Theorem 1.1.

Proof of (a) $\Longrightarrow$ (e) *in Theorem 1.1.* Let Ω be a domain of class $\mathscr{C}^{1+\alpha}$, $\alpha \in (0, 1)$, with compact boundary (hence, in particular, Ω is a UR domain). Also, assume $P(x)$ is an odd, homogeneous, harmonic polynomial of degree $l \geq 1$ in $\mathbb{R}^n$ and associate to it the singular integral operator

$$\mathbb{T}f(x) := \int_{\partial\Omega} \frac{P(x-y)}{|x-y|^{n-1+l}} f(y)\,d\sigma(y), \qquad x \in \Omega. \tag{6-1}$$

In a first stage, the goal is to prove that there exists a constant $C \in (1, \infty)$, depending only on n, α, $\mathrm{diam}(\partial\Omega)$, $\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)}$ and the upper Ahlfors regularity constant of $\partial\Omega$ (something we shall indicate by writing $C = C(n, \alpha, \Omega)$), such that for every $f \in \mathscr{C}^\alpha(\partial\Omega)$ we have

$$\sup_{x\in\Omega} |\mathbb{T}f(x)| + \sup_{x\in\Omega}\big\{\rho(x)^{1-\alpha}|\nabla(\mathbb{T}f)(x)|\big\} \leq C^l 2^{l^2} \|P\|_{L^1(S^{n-1})}\|f\|_{\mathscr{C}^\alpha(\partial\Omega)}. \tag{6-2}$$

We shall do so by induction on $l \in 2\mathbb{N}-1$, the degree of the homogeneous harmonic polynomial P. When $l = 1$ we have $P(x) = \sum_{j=1}^n a_j x_j$ for each $x = (x_1, \dots, x_n) \in \mathbb{R}^n$, where the a_j are some fixed constants. Hence, in this case,

$$\max_{1\leq j\leq n} |a_j| \leq \|P\|_{L^\infty(S^{n-1})} \leq c_n\|P\|_{L^1(S^{n-1})}, \tag{6-3}$$

where the last inequality is a consequence of (4-35) (with $c_n \in (0, \infty)$ denoting a dimensional constant), and

$$\mathbb{T} = \omega_{n-1}\sum_{j=1}^n a_j \partial_j \mathscr{S}. \tag{6-4}$$

Then (6-2) follows from (6-3), (6-4) and Lemmas 5.7 and 3.5. To proceed, fix some odd integer $l \geq 3$ and assume that there exists $C = C(n, \alpha, \Omega) \in (1, \infty)$ such that:

> The estimate in (6-2) holds whenever $\mathbb{T}$ is associated as in (6-1) with an odd harmonic homogeneous polynomial of degree at most $l-2$ in $\mathbb{R}^n$. (6-5)

Also, pick an arbitrary odd harmonic homogeneous polynomial $P(x)$ of degree l in $\mathbb{R}^n$ and let $\mathbb{T}$ be as in (6-1) for this choice of P. Consider the family $P_{rs}(x)$, $1 \leq r, s \leq n$, of odd harmonic homogeneous polynomials of degree $l-2$, as well as the family of odd $\mathscr{C}^\infty$ functions $k_{rs}:\mathbb{R}^n\setminus\{0\}\to\mathbb{R}^n\hookrightarrow \mathcal{C}\ell_n$, associated with P as in Lemma 4.2. For each $1\le i,\ j\le n$ set

$$k^{rs}(x) := \frac{P_{rs}(x)}{|x|^{n+l-3}} \quad \text{for } x\in\mathbb{R}^n\setminus\{0\}, \tag{6-6}$$

and introduce the integral operator, acting on Clifford algebra-valued functions $f=\sum_I f_I e_I$ with Hölder scalar components f_I defined on $\partial\Omega$,

$$\mathbb{T}^{rs} f(x) := \int_{\partial\Omega} k^{rs}(x-y)f(y)\,d\sigma(y) = \sum_I \biggl(\int_{\partial\Omega} k^{rs}(x-y)f_I(y)\,d\sigma(y)\biggr)e_I, \quad x\in\Omega. \tag{6-7}$$

Fix such an arbitrary $f\in\mathscr{C}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n$. Then, from the properties of the P_{rs} and the induction hypothesis (6-5) (used component-wise, keeping in mind that the sum in (6-7) is performed over a set of cardinality 2^n), we conclude that for each $1\le r,s\le n$ we have

$$\begin{aligned}\sup_{x\in\Omega}|(\mathbb{T}^{rs}f)(x)| + \sup_{x\in\Omega}\bigl\{\rho(x)^{1-\alpha}|\nabla(\mathbb{T}^{rs}f)(x)|\bigr\} &\le 2^{n/2}C^{l-2}2^{(l-2)^2}\|P_{rs}\|_{L^1(S^{n-1})}\|f\|_{\mathscr{C}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n}\\ &\le c_n C^{l-2}2^{(l-2)^2}2^l\|P\|_{L^1(S^{n-1})}\|f\|_{\mathscr{C}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n}.\end{aligned} \tag{6-8}$$

Moving on, for every $r,s\in\{1,\dots,n\}$ and $f:\partial\Omega\to\mathcal{C}\ell_n$ with Hölder scalar components, we set

$$\mathbb{T}_{rs}f(x) := \int_{\partial\Omega} k_{rs}(x-y)\odot f(y)\,d\sigma(y), \quad x\in\Omega. \tag{6-9}$$

Then, thanks to (4-23), whenever the function f is actually scalar-valued (i.e., $f:\partial\Omega\to\mathbb{R}\hookrightarrow\mathcal{C}\ell_n$) the original operator $\mathbb{T}$ from (6-1) may be recovered from the above $\mathbb{T}_{rs}$ by means of the identity

$$\mathbb{T}f(x) = \sum_{r,s=1}^n [\mathbb{T}_{rs}f(x)]_s \quad \text{for all } x\in\Omega. \tag{6-10}$$

To proceed, consider first the case when Ω is unbounded. In this scenario, fix some $x\in\Omega$ and select

$$R_1\in(0,\operatorname{dist}(x,\partial\Omega)) \quad\text{and}\quad R_2>\operatorname{dist}(x,\partial\Omega)+\operatorname{diam}(\partial\Omega). \tag{6-11}$$

Set $\Omega_{R_1,R_2} := (B(x,R_2)\setminus\overline{B(x,R_1)})\cap\Omega$, which is a bounded $\mathscr{C}^{1+\alpha}$ domain in $\mathbb{R}^n$ with the property that

$$\partial\Omega_{R_1,R_2} = \partial B(x,R_2)\cup\partial B(x,R_1)\cup\partial\Omega. \tag{6-12}$$

We continue to denote by ν and σ the outward unit normal and surface measure for Ω_{R_1,R_2}. As a consequence of (4-18) (used with Ω_{R_1,R_2} in place of Ω, $u=k_{rs}(x-\cdot)\in\mathscr{C}^\infty(\overline{\Omega}_{R_1,R_2})$ and $v\equiv 1$)

and (4-24), we then obtain that, for each $r, s \in \{1, \dots, n\}$,

$$\begin{aligned}\int_{\partial\Omega_{R_1,R_2}} k_{rs}(x-y)\odot\nu(y)\,d\sigma(y) &= -\int_{\Omega_{R_1,R_2}} (D_R k_{rs})(x-y)\,dy\\ &= \frac{l-1}{n+l-3}\int_{\Omega_{R_1,R_2}} \frac{\partial}{\partial y_r}\Big(\frac{P_{rs}(x-y)}{|x-y|^{n+l-3}}\Big)\,dy\\ &= \frac{l-1}{n+l-3}\int_{\partial\Omega_{R_1,R_2}} k^{rs}(x-y)\nu_r(y)\,d\sigma(y). \end{aligned}\tag{6-13}$$

Hence,

$$\begin{aligned}(\mathbb{T}_{rs}\nu)(x) &= \int_{\partial\Omega} k_{rs}(x-y)\odot\nu(y)\,d\sigma(y)\\ &= \int_{\partial\Omega_{R_1,R_2}} k_{rs}(x-y)\odot\nu(y)\,d\sigma(y) - \int_{\partial B(x,R_1)} k_{rs}(x-y)\odot\frac{x-y}{|x-y|}\,d\sigma(y)\\ &\qquad + \int_{\partial B(x,R_2)} k_{rs}(x-y)\odot\frac{x-y}{|x-y|}\,d\sigma(y)\\ &= \frac{l-1}{n+l-3}\int_{\partial\Omega_{R_1,R_2}} k^{rs}(x-y)\nu_r(y)\,d\sigma(y) - \int_{S^{n-1}} k_{rs}(\omega)\odot\omega\,d\omega + \int_{S^{n-1}} k_{rs}(\omega)\odot\omega\,d\omega\\ &= \frac{l-1}{n+l-3}\int_{\partial\Omega} k^{rs}(x-y)\nu_r(y)\,d\sigma(y) - \frac{l-1}{n+l-3}\int_{\partial B(x,R_1)} k^{rs}(x-y)\frac{x_r-y_r}{|x-y|}\,d\sigma(y)\\ &\qquad + \frac{l-1}{n+l-3}\int_{\partial B(x,R_2)} k^{rs}(x-y)\frac{x_r-y_r}{|x-y|}\,d\sigma(y)\\ &= \frac{l-1}{n+l-3}(\mathbb{T}^{rs}\nu_r)(x) - \frac{l-1}{n+l-3}\int_{S^{n-1}} k^{rs}(\omega)\omega_r\,d\omega + \frac{l-1}{n+l-3}\int_{S^{n-1}} k^{rs}(\omega)\omega_r\,d\omega\\ &= \frac{l-1}{n+l-3}(\mathbb{T}^{rs}\nu_r)(x). \end{aligned}\tag{6-14}$$

From (6-14) and (6-8) used with $f = \nu_r \in \mathscr{C}^\alpha(\partial\Omega)$, for $1 \le r, s \le n$ we obtain

$$\begin{aligned}\sup_{x\in\Omega}|(\mathbb{T}_{rs}\nu)(x)| + \sup_{x\in\Omega}\big\{\rho(x)^{1-\alpha}|\nabla(\mathbb{T}_{rs}\nu)(x)|\big\} &\le \sup_{x\in\Omega}|(\mathbb{T}^{rs}\nu_r)(x)| + \sup_{x\in\Omega}\big\{\rho(x)^{1-\alpha}|\nabla(\mathbb{T}^{rs}\nu_r)(x)|\big\}\\ &\le c_n C^{l-2} 2^{(l-2)^2} 2^l \|P\|_{L^1(S^{n-1})}\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)} \end{aligned}\tag{6-15}$$

in the case when Ω is an unbounded domain.

When Ω is a bounded domain, we once again consider Ω_{R_1,R_2} as before and carry out a computation similar in spirit to what we have just done above. This time, however, $\Omega_{R_1,R_2} = \Omega \setminus \overline{B(x, R_1)}$ and in place of (6-12) we have $\partial\Omega_{R_1,R_2} = \partial B(x, R_1) \cup \partial\Omega$. Consequently, in place of (6-14) we now obtain

$$(\mathbb{T}_{rs}\nu)(x) = \frac{l-1}{n+l-3}(\mathbb{T}^{rs}\nu_r)(x) - \frac{l-1}{n+l-3}\int_{S^{n-1}} k^{rs}(\omega)\omega_r\,d\omega - \int_{S^{n-1}} k_{rs}(\omega)\odot\omega\,d\omega. \tag{6-16}$$

To estimate the integrals on the unit sphere we note that, in view of (6-6), (4-26), (4-35) and (4-25), we have

$$\|k^{rs}\|_{L^\infty(S^{n-1})} + \|k_{rs}\|_{L^\infty(S^{n-1})} \le c_n 2^l \|P\|_{L^1(S^{n-1})}. \tag{6-17}$$

Upon observing that $\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)} \geq 1$, from (6-16) and (6-17) we deduce that an estimate similar to (6-15) also holds in the case when Ω is a bounded domain (this time replacing the constant c_n appearing in (6-15) by $2c_n$, which is inconsequential for our purposes). In summary, (6-16) may be assumed to hold whether Ω is bounded or not.

Going further, let $\widetilde{\mathbb{T}}_{rs}$ be the version of $\mathbb{T}_{rs}$ from (6-9) in which $\nu(y)$ has been absorbed into the integral kernel. That is, for $f : \partial\Omega \to \mathcal{C}\ell_n$ with Hölder scalar components set

$$\widetilde{\mathbb{T}}_{rs} f(x) := \int_{\partial\Omega} (k_{rs}(x-y) \odot \nu(y)) \odot f(y)\, d\sigma(y), \quad x \in \Omega, \tag{6-18}$$

for each $r, s \in \{1, \dots, n\}$. Since $\widetilde{\mathbb{T}}_{rs} 1 = \mathbb{T}_{rs}\nu$, from (6-15) we conclude that, for each $r, s \in \{1, \dots, n\}$,

$$\sup_{x\in\Omega} |(\widetilde{\mathbb{T}}_{rs}1)(x)| + \sup_{x\in\Omega}\bigl\{\rho(x)^{1-\alpha}|\nabla(\widetilde{\mathbb{T}}_{rs}1)(x)|\bigr\} \leq c_n C^{l-2} 2^{(l-2)^2} 2^l \|P\|_{L^1(S^{n-1})} \|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)}. \tag{6-19}$$

Given that the integral kernel of $\widetilde{\mathbb{T}}_{rs}$ satisfies

$$|k_{rs}(x-y) \odot \nu(y)| \leq \frac{\|k_{rs}\|_{L^\infty(S^{n-1})}}{|x-y|^{n-1}} \leq \frac{c_n 2^l \|P\|_{L^1(S^{n-1})}}{|x-y|^{n-1}}, \tag{6-20}$$

$$\bigl|\nabla_x [k_{rs}(x-y) \odot \nu(y)]\bigr| \leq \frac{\|\nabla k_{rs}\|_{L^\infty(S^{n-1})}}{|x-y|^{n}} \leq \frac{c_n 2^l \|P\|_{L^1(S^{n-1})}}{|x-y|^{n}}, \tag{6-21}$$

we may invoke Lemma 3.5 with

$$A := c_n C^{l-2} 2^{(l-2)^2} 2^l \|P\|_{L^1(S^{n-1})} \|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)} \quad \text{and} \quad B := c_n 2^l \|P\|_{L^1(S^{n-1})} \tag{6-22}$$

in order to conclude that if $1 \leq r, s \leq n$ then

$$\sup_{x\in\Omega} |\widetilde{\mathbb{T}}_{rs} f(x)| + \sup_{x\in\Omega}\bigl\{\rho(x)^{1-\alpha}|\nabla(\widetilde{\mathbb{T}}_{rs} f)(x)|\bigr\} \\ \leq C_{n,\alpha,\Omega}\{C^{l-2} 2^{(l-2)^2} 2^l \|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)} + 2^l\} \|P\|_{L^1(S^{n-1})} \|f\|_{\mathscr{C}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n} \tag{6-23}$$

for every $f \in \mathscr{C}^\alpha(\partial\Omega) \otimes \mathcal{C}\ell_n$. Writing (6-23) for f replaced by $\nu \odot f$ then yields — in light of (6-18), (6-9) and (4-21) (bearing in mind that $\nu \odot \nu = -1$) — that for $1 \leq r, s \leq n$ we have

$$\sup_{x\in\Omega} |\mathbb{T}_{rs} f(x)| + \sup_{x\in\Omega}\bigl\{\rho(x)^{1-\alpha}|\nabla(\mathbb{T}_{rs} f)(x)|\bigr\} \\ \leq C_{n,\alpha,\Omega}\{C^{l-2} 2^{(l-2)^2} 2^l \|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)} + 2^l\} \times 2\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)} \|P\|_{L^1(S^{n-1})} \|f\|_{\mathscr{C}^\alpha(\partial\Omega)\otimes\mathcal{C}\ell_n} \tag{6-24}$$

for every $f \in \mathscr{C}^\alpha(\partial\Omega) \otimes \mathcal{C}\ell_n$. In turn, from this and (6-10) we finally conclude that

$$\sup_{x\in\Omega} |\mathbb{T} f(x)| + \sup_{x\in\Omega}\bigl\{\rho(x)^{1-\alpha}|\nabla(\mathbb{T} f)(x)|\bigr\} \\ \leq n^2 C_{n,\alpha,\Omega}\{C^{l-2} 2^{(l-2)^2} 2^l \|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)} + 2^l\} \times 2\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)} \|P\|_{L^1(S^{n-1})} \|f\|_{\mathscr{C}^\alpha(\partial\Omega)} \tag{6-25}$$

for every $f \in \mathscr{C}^\alpha(\partial\Omega)$. Having established (6-25), we now see that (6-2) holds provided the constant $C \in (1, \infty)$ is chosen in such a way that

$$n^2 C_{n,\alpha,\Omega}\bigl\{C^{l-2} 2^{(l-2)^2} 2^l \|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)} + 2^l\bigr\} 2\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)} \leq C^l 2^{l^2} \tag{6-26}$$

for each odd number $l \in \mathbb{N}$, $l \geq 3$. Since $2^{(l-2)^2} 2^l \leq 2 \cdot 2^{l^2}$ and $2^l \leq C^{l-2} 2^{l^2}$, it follows that the left-hand side of (6-26) is at most $C(n, \alpha, \Omega) C^{l-2} 2^{l^2}$. This, in turn, is bounded by the right-hand side of (6-26) provided $C \geq \max\{1, \sqrt{C(n, \alpha, \Omega)}\}$. In summary, choosing such a C ensures that (6-2) holds.

Next, we aim to show that (6-2) continues to be valid if the harmonicity condition on P is dropped, that is, when

$$P(x) \text{ is a homogeneous polynomial in } \mathbb{R}^n \text{ of degree } l \in 2\mathbb{N} - 1. \tag{6-27}$$

Indeed, a standard fact about arbitrary homogeneous polynomials $P(x)$ is the decomposition (see [Stein 1970, §3.1.2, p. 69])

$$P(x) = P_1(x) + |x|^2 Q_1(x) \quad \text{for every } x \in \mathbb{R}^n, \tag{6-28}$$

where P_1 and Q_1 are homogeneous polynomials and P_1 is harmonic. Hence, if $P(x)$ is a homogeneous polynomial of degree $l = 2N+1$ in $\mathbb{R}^n$ for some $N \in \mathbb{N}_0$, not necessarily harmonic, then by iterating (6-28) we obtain

$$P(x) = \sum_{j=1}^{N+1} |x|^{2(j-1)} P_j(x) \quad \text{for every } x \in \mathbb{R}^n, \tag{6-29}$$

where each P_j is a harmonic homogeneous polynomial of degree $l - 2(j-1)$. Since the restrictions to the unit sphere of any two homogeneous harmonic polynomials of different degrees are orthogonal in $L^2(S^{n-1})$ (see [Stein 1970, §3.1.1, p. 69]), it follows from (6-29) that

$$\|P\|^2_{L^2(S^{n-1})} = \sum_{j=1}^{N+1} \|P_j\|^2_{L^2(S^{n-1})}. \tag{6-30}$$

In particular, for each j, Hölder's inequality and (6-30) permit us to estimate

$$\|P_j\|_{L^1(S^{n-1})} \leq c_n \|P_j\|_{L^2(S^{n-1})} \leq c_n \|P\|_{L^2(S^{n-1})}. \tag{6-31}$$

Combining (6-1) and (6-29), for any $x \in \Omega$ and $f \in \mathscr{C}^\alpha(\partial\Omega)$ we obtain

$$\mathbb{T} f(x) = \sum_{j=1}^{N+1} \int_{\partial\Omega} \frac{P_j(x-y)}{|x-y|^{n-1+(l-2(j-1))}} f(y)\, d\sigma(y), \tag{6-32}$$

and each integral operator appearing in the sum above is constructed according to the same blueprint as the original $\mathbb{T}$ in (6-1), including the property that the intervening homogeneous polynomial is harmonic. As such, repeated applications of (6-2) yield

$$\sup_{x\in\Omega} |\mathbb{T} f(x)| + \sup_{x\in\Omega} \bigl\{\rho(x)^{1-\alpha} |\nabla(\mathbb{T} f)(x)|\bigr\} \leq c_n l C^l 2^{l^2} \|P\|_{L^2(S^{n-1})} \|f\|_{\mathscr{C}^\alpha(\partial\Omega)} \tag{6-33}$$

for each $f \in \mathscr{C}^\alpha(\partial\Omega)$. Since if C is bigger than a suitable dimensional constant, we have $c_n l \leq C^l$ for all l, by eventually replacing C by C^2 in (6-33). Ultimately, with the help of Lemma 2.10 (while keeping (2-55) in mind), we deduce that (1-19) holds for $\mathbb{T}_+$ in Ω_+. That $\mathbb{T}_-$ also satisfies similar properties follows in a similar manner, working in Ω_- (in place of Ω_+), which is also a domain of class $\mathscr{C}^{1+\alpha}$ with compact boundary. □

Proof of (e) $\Longrightarrow$ (d) *in Theorem 1.1.* This is obvious, since the operators $\mathscr{R}_j^{\pm}$ from (1-17) are particular cases of those considered in (1-18). □

Proof of (d) $\Longrightarrow$ (a) *in Theorem 1.1.* Since we are currently assuming that Ω is a UR domain, Theorem 3.2 applies in $\Omega_{\pm}$ and yields (bearing (2-49) in mind) the jump formulas

$$(\mathscr{R}_j^{\pm} f\big|^{\rm nt}_{\partial\Omega_{\pm}})(x) = \mp\tfrac{1}{2}\nu_j(x)f(x) + \lim_{\varepsilon\to 0^+}\int_{\partial\Omega\setminus B(x,\varepsilon)} (\partial_j E_{\Delta})(x-y)f(y)\,d\sigma(y) \tag{6-34}$$

for each $f \in L^p(\partial\Omega,\sigma)$ with $p\in[1,\infty)$, each $j\in\{1,\dots,n\}$, and σ-a.e. $x\in\partial\Omega$. Hence, by (6-34) and (1-16), we have

$$\nu_j = \mathscr{R}_j^{-}1\big|_{\partial\Omega_-} - \mathscr{R}_j^{+}1\big|_{\partial\Omega_+} \in \mathscr{C}^{\alpha}(\partial\Omega) \quad \text{for all } j\in\{1,\dots,n\}. \tag{6-35}$$

Given the present background assumptions on Ω, Theorem 2.2 then gives that Ω is a $\mathscr{C}^{1+\alpha}$ domain. □

Proof of (a) $\Longrightarrow$ (c) *in Theorem 1.1.* Assume that Ω is a domain of class $\mathscr{C}^{1+\alpha}$, $\alpha\in(0,1)$, with compact boundary. Here, the task is to prove that the principal value singular integral operator T, originally defined in (1-15), is a well-defined, linear and bounded mapping from $\mathscr{C}^{\alpha}(\partial\Omega)$ into itself. In the process, we shall also show that (1-20) holds. Since (a) $\Longrightarrow$ (e) has already been established, we know that the singular integral operator (6-1) maps $\mathscr{C}^{\alpha}(\partial\Omega)$ boundedly into $\mathscr{C}^{\alpha}(\overline{\Omega})$ with

$$\|\mathbb{T}f\|_{\mathscr{C}^{\alpha}(\overline{\Omega})} \le C^l 2^{l^2}\|P\|_{L^2(S^{n-1})}\|f\|_{\mathscr{C}^{\alpha}(\partial\Omega)} \quad \text{for all } f\in\mathscr{C}^{\alpha}(\partial\Omega). \tag{6-36}$$

For starters, let us operate under the additional assumption that the homogeneous polynomial P is harmonic, and abbreviate

$$k(x) := \frac{P(x)}{|x|^{n-1+l}} \quad \text{for all } x\in\mathbb{R}^n\setminus\{0\}. \tag{6-37}$$

In this scenario, (4-37) gives that

$$\hat{k}(\xi) = \mathcal{F}_{x\to\xi}\left(\frac{P(x)}{|x|^{n+l-1}}\right) = \gamma_{n,l,1}\frac{P(\xi)}{|\xi|^{l+1}} \quad \text{for all } \xi\in\mathbb{R}^n\setminus\{0\}. \tag{6-38}$$

Moreover, a direct computation, using Stirling's approximation formula

$$\sqrt{2\pi}\,m^{m+1/2}e^{-m} \le m! \le e m^{m+1/2}e^{-m} \quad \text{for all } m\in\mathbb{N}, \tag{6-39}$$

shows that

$$\gamma_{n,l,1} = \begin{cases} O(l^{-(n-2)/2}) & \text{if } n \text{ is even},\\ O(l^{-(n-4)/2}) & \text{if } n \text{ is odd},\end{cases} \qquad \text{as } l\to\infty. \tag{6-40}$$

We continue by observing that, thanks to (4-35),

$$\sup_{x\in\partial\Omega}|P(\nu(x))| \le \|P\|_{L^\infty(S^{n-1})} \le c_n 2^l l^{-1}\|P\|_{L^1(S^{n-1})}. \tag{6-41}$$

Next we note that $|\nu(x)-\nu(y)|\ge\frac{1}{2}$ forces $|x-y|^{\alpha}\ge 1/(2\|\nu\|_{\mathscr{C}^{\alpha}(\partial\Omega)})$, which further implies

$$\frac{|P(\nu(x))-P(\nu(y))|}{|x-y|^{\alpha}} \le 4\|\nu\|_{\mathscr{C}^{\alpha}(\partial\Omega)}\|P\|_{L^\infty(S^{n-1})} \le c_n 2^l l^{-1}\|\nu\|_{\mathscr{C}^{\alpha}(\partial\Omega)}\|P\|_{L^1(S^{n-1})} \tag{6-42}$$

by virtue of (4-35), while, if $|\nu(x)-\nu(y)|\leq\frac{1}{2}$, the mean value theorem and (4-35) permit us to once again estimate

$$\frac{|P(\nu(x))-P(\nu(y))|}{|x-y|^\alpha}\leq\Big(\sup_{z\in[\nu(x),\nu(y)]}|(\nabla P)(z)|\Big)\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)}\leq\|\nabla P\|_{L^\infty(S^{n-1})}\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)}$$
$$\leq c_n 2^l l^{-1}\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)}\|P\|_{L^1(S^{n-1})}. \tag{6-43}$$

By combining (6-38) and (6-40)–(6-43) we therefore arrive at the conclusion that the mapping $\partial\Omega\to\mathbb{C}$, $x\mapsto\hat{k}(\nu(x))$, belongs to $\mathscr{C}^\alpha(\partial\Omega)$ and

the mapping $\partial\Omega\ni x\mapsto\hat{k}(\nu(x))$ belongs to $\mathscr{C}^\alpha(\partial\Omega)$ and $\|\hat{k}(\nu(\cdot))\|_{\mathscr{C}^\alpha(\partial\Omega)}\leq$ $c_n 2^l\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)}\|P\|_{L^1(S^{n-1})}$. (6-44)

Next, the assumptions on Ω imply (see the discussion in Section 2) that this is both a UR domain and a uniform domain. As such, Theorem 3.2 applies. Since $\mathbb{T}$ from (6-1) corresponds to the operator $\mathcal{T}$ defined in (3-9) with k as in (6-37), for each $f\in\mathscr{C}^\alpha(\partial\Omega)$ we obtain from (3-12), (6-44), and (6-36) that

$$\begin{aligned}\|Tf\|_{\mathscr{C}^\alpha(\partial\Omega)}&\leq\big\|\tfrac{1}{2i}\hat{k}(\nu(\cdot))f+Tf\big\|_{\mathscr{C}^\alpha(\partial\Omega)}+\big\|\tfrac{1}{2i}\hat{k}(\nu(\cdot))f\big\|_{\mathscr{C}^\alpha(\partial\Omega)}\\&\leq\|\mathbb{T}f\big|^{\rm nt}_{\partial\Omega}\|_{\mathscr{C}^\alpha(\partial\Omega)}+2^{-1}\|\hat{k}(\nu(\cdot))\|_{\mathscr{C}^\alpha(\partial\Omega)}\|f\|_{\mathscr{C}^\alpha(\partial\Omega)}\\&=\|\mathbb{T}f|_{\partial\Omega}\|_{\mathscr{C}^\alpha(\partial\Omega)}+c_n2^l\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)}\|P\|_{L^1(S^{n-1})}\|f\|_{\mathscr{C}^\alpha(\partial\Omega)}\\&\leq\|\mathbb{T}f\|_{\mathscr{C}^\alpha(\bar{\Omega})}+c_n2^l\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)}\|P\|_{L^2(S^{n-1})}\|f\|_{\mathscr{C}^\alpha(\partial\Omega)}\\&\leq\{C^l2^{l^2}+c_n2^l\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)}\}\|P\|_{L^2(S^{n-1})}\|f\|_{\mathscr{C}^\alpha(\partial\Omega)}\\&\leq(C^2)^l2^{l^2}\|P\|_{L^2(S^{n-1})}\|f\|_{\mathscr{C}^\alpha(\partial\Omega)},\end{aligned}\tag{6-45}$$

assuming, without loss of generality, that $C\geq 2+c_n\|\nu\|_{\mathscr{C}^\alpha(\partial\Omega)}$ to begin with. Note that the estimate just derived has the format demanded in (1-20).

To treat the general case, when P is merely as in (6-27), consider the decomposition (6-29) and, for each $f\in\mathscr{C}^\alpha(\partial\Omega)$, write

$$Tf(x)=\sum_{j=1}^{N+1}\lim_{\varepsilon\to0^+}\int_{\substack{y\in\partial\Omega\\|x-y|>\varepsilon}}\frac{P_j(x-y)}{|x-y|^{n-1+(l-2(j-1))}}f(y)\,d\sigma(y),\quad x\in\partial\Omega. \tag{6-46}$$

Since every integral operator appearing in the right-hand side of (6-46) is of the same type as the original T in (1-15), with the additional property that the intervening homogeneous polynomial is harmonic, repeated applications of (6-45) give

$$\|Tf\|_{\mathscr{C}^\alpha(\partial\Omega)}\leq l(C^2)^l2^{l^2}\|P\|_{L^2(S^{n-1})}\|f\|_{\mathscr{C}^\alpha(\partial\Omega)}\quad\text{for all } f\in\mathscr{C}^\alpha(\partial\Omega). \tag{6-47}$$

Using $l\leq(C^2)^l$ for all l if C is sufficiently large and relabelling C^4 simply as C, the estimate (1-20) finally follows. □

Proof of (c) $\Longrightarrow$ (b) *in Theorem 1.1.* Observe that the principal value Riesz transforms $R_j^{\rm pv}$ from (1-1) with $\Sigma:=\partial\Omega$ are special cases of the principal value singular integral operators defined in (1-15) (corresponding to P as in (1-21)). Hence, on the one hand, $R_j^{\mathrm{pv}}1 \in \mathscr{C}^\alpha(\partial\Omega)$. On the other hand, since Ω is presently assumed to be a UR domain, from (1-13) it follows that each of the distributional Riesz transforms R_j from (1-4)–(1-5) with $\Sigma := \partial\Omega$ agrees with R_j^{pv} on $\mathscr{C}^\alpha(\partial\Omega)$. Combining these, we conclude that (1-14) holds. □

Proof of (b) $\Longrightarrow$ (a) *in Theorem 1.1.* Granted the background hypotheses on Ω, the assumption made in (1-14) allows us to invoke the $T(1)$ theorem (for operators associated with odd kernels, on spaces of homogeneous type). Thanks to this, (2-24) and the Calderón–Zygmund machinery mentioned earlier, we conclude that each of the distributional Riesz transforms R_j from (1-4)–(1-5) with $\Sigma := \partial\Omega$ extends to a bounded linear operator on $L^2(\partial\Omega)$, in the form of the principal value Riesz transform R_j^{pv} from (1-1) with $\Sigma := \partial\Omega$. In particular, we now have

$$R_j 1 = R_j^{\mathrm{pv}} 1 \quad \text{in } L^2(\partial\Omega). \tag{6-48}$$

Next observe that, since $\nu \odot \nu = -1$ at σ-a.e. point on $\partial\Omega$ and $x - y = \sum_{j=1}^n (x_j - y_j) e_j$ for every $x, y \in \mathbb{R}^n$, from (5-2), (1-1) and (6-48) we obtain

$$\mathcal{C}^{\mathrm{pv}} \nu = -\sum_{j=1}^n (R_j^{\mathrm{pv}} 1) e_j = \sum_{j=1}^n (R_j 1) e_j \quad \text{at } \sigma\text{-a.e. point on } \partial\Omega, \tag{6-49}$$

which, on account of (5-5), further yields

$$\tfrac{1}{4}\nu = \mathcal{C}^{\mathrm{pv}}(\mathcal{C}^{\mathrm{pv}}\nu) = -\mathcal{C}^{\mathrm{pv}}\biggl(\sum_{j=1}^n (R_j 1) e_j\biggr) \quad \text{at } \sigma\text{-a.e. point on } \partial\Omega. \tag{6-50}$$

With this in hand, it readily follows from Theorem 5.6 that if condition (1-14) holds then $\nu \in \mathscr{C}^\alpha(\partial\Omega)$. Having established this, Theorem 2.2 applies and gives that Ω is a domain of class $\mathscr{C}^{1+\alpha}$. □

This concludes the proof of Theorem 1.1, and we now turn to the proof of Theorem 1.3.

Proof of Theorem 1.3. This is a direct consequence of Proposition 2.12 and Corollary 1.2 upon observing that $\mathfrak{C}^{\mathrm{pv}} = i R_1^{\mathrm{pv}} + R_2^{\mathrm{pv}}$, where R_j^{pv}, $j = 1, 2$, are the two principal value Riesz transforms in the plane. □

We finally present the proof of Theorem 1.6.

Proof of Theorem 1.6. Let

$$k|_{S^{n-1}} = \sum_{l=0}^\infty Y_l \tag{6-51}$$

be the decomposition of $k|_{S^{n-1}} \in L^2(S^{n-1})$ in surface spherical harmonics. That is, $\{Y_l\}_{l\in\mathbb{N}_0}$ are mutually orthogonal functions in $L^2(S^{n-1})$ with the property that for each $l \in \mathbb{N}_0$ the function

$$P_l(x) := \begin{cases} |x|^l Y_l(x/|x|) & \text{if } x \in \mathbb{R}^n \setminus \{0\}, \\ 0 & \text{if } x = 0, \end{cases} \tag{6-52}$$

is a homogeneous harmonic polynomial of degree l in $\mathbb{R}^n$. In particular,

$$\Delta_{S^{n-1}} Y_l = -l(l+n-2) Y_l \quad \text{on } S^{n-1} \text{ for all } l \in \mathbb{N}_0. \tag{6-53}$$

See, for example, [Stein 1970, pp. 68–70] for a discussion. Then, for each $l \in \mathbb{N}_0$, we may write

$$\begin{aligned}[-l(l+n-2)]^{m_l}\|Y_l\|^2_{L^2(S^{n-1})} &= [-l(l+n-2)]^{m_l}\int_{S^{n-1}} k\overline{Y}_l\,d\omega \\ &= \int_{S^{n-1}} k\Delta^{m_l}_{S^{n-1}}\overline{Y}_l\,d\omega = \int_{S^{n-1}} (\Delta^{m_l}_{S^{n-1}}k)\overline{Y}_l\,d\omega, \end{aligned} \tag{6-54}$$

where the first equality uses (6-51), the second one is based on (6-53), and the third one follows via repeated integrations by parts. In turn, from (6-54) and the Cauchy–Schwarz inequality we obtain

$$\|Y_l\|_{L^2(S^{n-1})} \le l^{-2m_l}\|\Delta^{m_l}_{S^{n-1}}k\|_{L^2(S^{n-1})} \quad \text{for all } l \in \mathbb{N}_0. \tag{6-55}$$

We continue by noting that the homogeneity of k together with (6-51) and (6-52) permit us to express

$$k(x) = \frac{k(x/|x|)}{|x|^{n-1}} = \sum_{l=0}^{\infty}\frac{Y_l(x/|x|)}{|x|^{n-1}} = \sum_{l=0}^{\infty}\frac{P_l(x/|x|)}{|x|^{n-1}} = \sum_{l=0}^{\infty}\frac{P_l(x)}{|x|^{n-1+l}} \tag{6-56}$$

for each $x \in \mathbb{R}^n \setminus \{0\}$. For each $l \in \mathbb{N}_0$, let $\mathbb{T}_l$ and T_l be the integral operators defined analogously to (1-32) and (1-33) in which the kernel $k(x-y)$ has been replaced by $P_l(x-y)|x-y|^{-(n-1+l)}$. Then, for each $f \in \mathscr{C}^\alpha(\partial\Omega)$, we may estimate

$$\begin{aligned}\sum_{l=0}^{\infty}\|\mathbb{T}_l f\|_{\mathscr{C}^\alpha(\overline{\Omega})} &\le \sum_{l=0}^{\infty} C^l 2^{l^2}\|P_l\|_{L^2(S^{n-1})}\|f\|_{\mathscr{C}^\alpha(\partial\Omega)} \\ &= \sum_{l=0}^{\infty} C^l 2^{l^2}\|Y_l\|_{L^2(S^{n-1})}\|f\|_{\mathscr{C}^\alpha(\partial\Omega)} \\ &\le \biggl(\sum_{l=0}^{\infty} C^l 2^{l^2} l^{-2m_l}\|\Delta^{m_l}_{S^{n-1}}k\|_{L^2(S^{n-1})}\biggr)\|f\|_{\mathscr{C}^\alpha(\partial\Omega)}, \end{aligned} \tag{6-57}$$

by invoking (1-19) and (6-55), and keeping in mind that $P|_{S^{n-1}} = Y_l$ (see (6-52)). Since for l large we have $C^l 2^{l^2} \le 4^{l^2}$, it follows from (1-31) that the series in the curly bracket in (6-57) is convergent to some finite constant M. Based on this and (6-56), we may then conclude that $\|\mathbb{T}f\|_{\mathscr{C}^\alpha(\overline{\Omega})} \le \sum_{l=0}^{\infty}\|\mathbb{T}_l f\|_{\mathscr{C}^\alpha(\overline{\Omega})} \le M\|f\|_{\mathscr{C}^\alpha(\partial\Omega)}$. This proves the boundedness of the first operator in (1-34), and the second operator in (1-34) is treated similarly (making use of (1-20)). □

Remark 6.1. We claim that (1-31) is satisfied whenever the kernel k is of the form $P(x)/|x|^{n-1+l_o}$ for some homogeneous polynomial P of degree $l_o \in 2\mathbb{N}-1$ in $\mathbb{R}^n$. Indeed, writing $P(x)/|x|^{n-1+l_o} = P(x/|x|)/|x|^{n-1}$ and invoking (6-29), there is no loss of generality in assuming that P is also harmonic to begin with. Granted this, it follows that $k|_{S^{n-1}} = P|_{S^{n-1}}$ is a surface spherical harmonic of degree l_o; hence — see [Stein 1970, §3.1.4, p. 70] — $\Delta_{S^{n-1}}(k|_{S^{n-1}}) = -l_o(l_o+n-2)(k|_{S^{n-1}})$. Choosing $m_l := l^2$ for each $l \in \mathbb{N}_0$ and iterating this formula then shows that the series in (1-31) is dominated by

$$\sum_{l=0}^{\infty} 4^{l^2} l^{-2l^2}[l_o(l_o+n-2)]^{l^2}\|k\|_{L^2(S^{n-1})} < +\infty. \tag{6-58}$$

7. Further results

We start by recalling some definitions. First, given a compact Ahlfors regular set $\Sigma \subset \mathbb{R}^n$, introduce $\sigma := \mathcal{H}^{n-1}\lfloor\Sigma$ and define the John–Nirenberg space of functions of bounded mean oscillations on Σ as

$$\mathrm{BMO}(\Sigma) := \{f \in L^1(\Sigma, \sigma) : f^{\#,p} \in L^\infty(\Sigma, \sigma)\}, \tag{7-1}$$

where $p \in [1, \infty)$ is a fixed parameter and

$$f^{\#,p}(x) := \sup_{r>0}\left(\frac{1}{\sigma(\Sigma \cap B(x,r))}\int_{\Sigma\cap B(x,r)} |f(y) - f_{\Delta(x,r)}|^p \, d\sigma(y)\right)^{\frac{1}{p}}, \tag{7-2}$$

with $f_{\Delta(x,r)}$ the mean value of f on $\Sigma \cap B(x,r)$. As is well known, various choices of p give the same space. Keeping this in mind, we define the seminorm

$$[f]_{\mathrm{BMO}(\Sigma)} := \|f^{\#,p}\|_{L^\infty(\Sigma,\sigma)}. \tag{7-3}$$

We then define the Sarason space $\mathrm{VMO}(\Sigma)$ of functions of vanishing mean oscillations on Σ as the closure in $\mathrm{BMO}(\Sigma)$ of $\mathscr{C}^0(\Sigma)$, the space of continuous functions on Σ. Alternatively, given any $\alpha \in (0, 1)$, the space $\mathrm{VMO}(\Sigma)$ may be described (see [Hofmann et al. 2010, Proposition 2.15, p. 2602]) as the closure in $\mathrm{BMO}(\Sigma)$ of $\mathscr{C}^\alpha(\Sigma)$. Hence, in the present context,

$$\bigcup_{0\le\alpha<1} \mathscr{C}^\alpha(\Sigma) \hookrightarrow \mathrm{VMO}(\Sigma) \hookrightarrow \mathrm{BMO}(\Sigma) \hookrightarrow \bigcap_{0<p<\infty} L^p(\Sigma, \sigma). \tag{7-4}$$

Proposition 7.1. *If $\Omega \subseteq \mathbb{R}^n$ is a* UR *domain with compact boundary then the principal value Cauchy–Clifford operator $\mathcal{C}^{\mathrm{pv}}$ from* (5-2) *is bounded both on $\mathrm{BMO}(\partial\Omega)\otimes \mathcal{C}\ell_n$ and on $\mathrm{VMO}(\partial\Omega)\otimes\mathcal{C}\ell_n$. Moreover, $(\mathcal{C}^{\mathrm{pv}})^2 = \frac{1}{4}I$ both on $\mathrm{BMO}(\partial\Omega)\otimes\mathcal{C}\ell_n$ and on $\mathrm{VMO}(\partial\Omega)\otimes\mathcal{C}\ell_n$. Hence, in particular, $\mathcal{C}^{\mathrm{pv}}$ is an isomorphism when acting on either of these spaces.*

Proof. To begin with, observe that in the present setting (5-21) ensures that $\mathcal{C}^{\mathrm{pv}}$ is well-defined on $\mathrm{BMO}(\partial\Omega)\otimes\mathcal{C}\ell_n$. Now fix $f \in \mathrm{BMO}(\partial\Omega)\otimes\mathcal{C}\ell_n$ and pick some $x_0 \in \partial\Omega$ and $r > 0$. For each $R > 0$, let us agree to abbreviate $\Delta_R := \partial\Omega \cap B(x_0, R)$. Denote by ν the geometric measure-theoretic outward unit normal to Ω and, with $\sigma := \mathcal{H}^{n-1}\lfloor\partial\Omega$, introduce

$$A(x_0, r) := \frac{1}{\omega_{n-1}}\int_{\substack{y\in\partial\Omega\\ |x_0-y|\ge 2r}} \frac{x_0 - y}{|x_0 - y|^n} \odot \nu(y) \odot (f(y) - f_{\Delta_{2r}})\, d\sigma(y) \pm \tfrac{1}{2} f_{\Delta_{2r}}, \tag{7-5}$$

where the sign is chosen to be plus if Ω is bounded and minus if Ω is unbounded, and where $f_{\Delta_{2r}}$ stands for the integral average of f over Δ_{2r}. For $x \in \Delta_r$, use (5-21) to split

$$\begin{aligned}\mathcal{C}^{\mathrm{pv}} f(x) = \lim_{\varepsilon\to 0^+} \frac{1}{\omega_{n-1}}\int_{\substack{y\in\partial\Omega\setminus B(x,\varepsilon)\\ |x_0-y|<2r}} \frac{x-y}{|x-y|^n} \odot \nu(y) \odot (f(y) - f_{\Delta_{2r}})\, d\sigma(y)\\ + \frac{1}{\omega_{n-1}}\int_{\substack{y\in\partial\Omega\\ |x_0-y|\ge 2r}} \left(\frac{x-y}{|x-y|^n} - \frac{x_0-y}{|x_0-y|^n}\right)\odot\nu(y)\odot(f(y)-f_{\Delta_{2r}})\, d\sigma(y) + A(x_0, r),\end{aligned} \tag{7-6}$$

then employ this representation (and Minkowski's inequality) in order to estimate

$$\left(\frac{1}{\sigma(\Delta_r)}\int_{\Delta_r}|\mathcal{C}^{\mathrm{pv}}f(x)-A(x_0,r)|^2\,d\sigma(x)\right)^{\frac{1}{2}}\le c(I+II), \tag{7-7}$$

where $c\in(0,\infty)$ depends only on Ω and

$$\begin{aligned} I &:= \left(\frac{1}{\sigma(\Delta_r)}\int_{\partial\Omega}|\mathcal{C}^{\mathrm{pv}}((f-f_{\Delta_{2r}})\mathbf{1}_{\Delta_{2r}})|^2\,d\sigma\right)^{\frac{1}{2}},\\ II &:= r^{-n-1/(2)}\int_{\substack{y\in\partial\Omega\\ |x_0-y|\ge 2r}}\left(\int_{\Delta_r}\left|\frac{x-y}{|x-y|^n}-\frac{x_0-y}{|x_0-y|^n}\right|^2 d\sigma(x)\right)^{\frac{1}{2}}|f(y)-f_{\Delta_{2r}}|\,d\sigma(y). \end{aligned}$$

Now, the boundedness of $\mathcal{C}^{\mathrm{pv}}$ on $L^2(\partial\Omega,\sigma)\otimes\mathcal{C}\ell_n$ from Proposition 5.1 gives (bearing in mind that σ is doubling)

$$I\le c\left(\frac{1}{\sigma(\Delta_{2r})}\int_{\Delta_{2r}}|f-f_{\Delta_{2r}}|^2\,d\sigma\right)^{\frac{1}{2}}\le c[f]_{\mathrm{BMO}(\partial\Omega)\otimes\mathcal{C}\ell_n}, \tag{7-8}$$

which suits our purposes. Next, we write

$$\begin{aligned} II &\le c\int_{\substack{y\in\partial\Omega\\ |x_0-y|\ge 2r}}\frac{r}{|x_0-y|^n}|f(y)-f_{\Delta_{2r}}|\,d\sigma(y)\\ &\le c\sum_{j=1}^{\infty}\int_{\Delta_{2^{j+1}r}\setminus\Delta_{2^j r}}\frac{r}{(2^j r)^n}|f(y)-f_{\Delta_{2r}}|\,d\sigma(y)\\ &\le c\sum_{j=1}^{\infty}\frac{1}{2^j}\fint_{\Delta_{2^{j+1}r}}|f-f_{\Delta_{2r}}|\,d\sigma\\ &\le c\sum_{j=1}^{\infty}\frac{1}{2^j}\fint_{\Delta_{2^{j+1}r}}\left[|f-f_{\Delta_{2^{j+1}r}}|+\sum_{k=1}^{j}|f_{\Delta_{2^{k+1}r}}-f_{\Delta_{2^k r}}|\right]d\sigma\\ &\le c\sum_{j=1}^{\infty}\frac{1}{2^j}(1+j)f^{\#,1}(x_0)\le cf^{\#,1}(x_0)\le c[f]_{\mathrm{BMO}(\partial\Omega)\otimes\mathcal{C}\ell_n}. \end{aligned} \tag{7-9}$$

Above, the first inequality follows from the mean value theorem, while the second inequality is a consequence of writing the integral over $\partial\Omega\setminus\Delta_{2r}$ as the telescopic sum over $\Delta_{2^{j+1}r}\setminus\Delta_{2^j r}$, $j\in\mathbb{N}$, and the fact that $|x_0-y|\ge 2^j r$ for $y\in\Delta_{2^{j+1}r}\setminus\Delta_{2^j r}$. The third inequality is a result of enlarging the domain of integration from $\Delta_{2^{j+1}r}\setminus\Delta_{2^j r}$ to $\Delta_{2^{j+1}r}$ and using $\sigma\big(\Delta_{2^{j+1}r}\big)\approx(2^j r)^{n-1}$. The fourth inequality follows from the triangle inequality after writing

$$f-f_{\Delta_{2r}}=f-f_{\Delta_{2^{j+1}r}}+\sum_{k=1}^{j}(f_{\Delta_{2^{k+1}r}}-f_{\Delta_{2^k r}}). \tag{7-10}$$

The fifth inequality is a consequence of the fact that, for each k, we have

$$|f_{\Delta_{2^{k+1}r}} - f_{\Delta_{2^k r}}| = \left| ⨍_{\Delta_{2^k r}} (f - f_{\Delta_{2^{k+1}r}})\, d\sigma \right| \leq c ⨍_{\Delta_{2^{k+1}r}} |f - f_{\Delta_{2^{k+1}r}}|\, d\sigma \leq c\, f^{\#,1}(x_0). \tag{7-11}$$

The sixth inequality is a consequence of $\sum_{j=1}^{\infty} 2^{-j}(1+j) < +\infty$ and, finally, the last inequality is seen from (7-3).

From (7-7)–(7-9) we eventually obtain $\|(\mathcal{C}^{\mathrm{pv}} f)^{\#,2}\|_{L^\infty(\partial\Omega,\sigma)\otimes\mathcal{C}\ell_n} \leq c[f]_{\mathrm{BMO}(\partial\Omega)\otimes\mathcal{C}\ell_n}$; hence,

$$[\mathcal{C}^{\mathrm{pv}} f]_{\mathrm{BMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} \leq c[f]_{\mathrm{BMO}(\partial\Omega)\otimes\mathcal{C}\ell_n}, \tag{7-12}$$

from which we conclude that the operator

$$\mathcal{C}^{\mathrm{pv}} : \mathrm{BMO}(\partial\Omega) \otimes \mathcal{C}\ell_n \longrightarrow \mathrm{BMO}(\partial\Omega) \otimes \mathcal{C}\ell_n \tag{7-13}$$

is well-defined and bounded. Next, that

$$\mathcal{C}^{\mathrm{pv}} : \mathrm{VMO}(\partial\Omega) \otimes \mathcal{C}\ell_n \longrightarrow \mathrm{VMO}(\partial\Omega) \otimes \mathcal{C}\ell_n \tag{7-14}$$

is also well-defined and bounded follows from (7-13), the characterization of $\mathrm{VMO}(\partial\Omega) \otimes \mathcal{C}\ell_n$ as the closure in $\mathrm{BMO}(\partial\Omega) \otimes \mathcal{C}\ell_n$ of $\mathscr{C}^\alpha(\partial\Omega) \otimes \mathcal{C}\ell_n$ for each $\alpha \in (0, 1)$, and Theorem 5.6.

Finally, the claims in the last part of the statement of the proposition are direct consequences of what we have proved so far, (7-4), and (5-5). □

When $\Omega \subseteq \mathbb{R}^n$ is a UR domain with compact boundary, it follows from (1-13) and (3-8) in Theorem 3.1 that R_j maps $\mathscr{C}^\alpha(\partial\Omega)$ into $\mathrm{BMO}(\partial\Omega)$ for each $j \in \{1, \dots, n\}$. Hence, in this case, $R_j 1 \in \mathrm{BMO}(\partial\Omega)$ for each $j \in \{1, \dots, n\}$. Remarkably, the proximity of the BMO functions $R_j 1$, $1 \leq j \leq n$, to the space $\mathrm{VMO}(\partial\Omega)$ controls how close the outward unit normal ν to Ω is to being in $\mathrm{VMO}(\partial\Omega)$. Specifically, we have the following result:

Theorem 7.2. *Let $\Omega \subseteq \mathbb{R}^n$ be a* UR *domain with compact boundary and denote by ν the geometric measure-theoretic outward unit normal to Ω. Also, let $\|\mathcal{C}^{\mathrm{pv}}\|_*$ stand for the operator norm of the Cauchy–Clifford singular integral operator acting on the space* $\mathrm{BMO}(\partial\Omega) \otimes \mathcal{C}\ell_n$. *Then, with distances considered in* $\mathrm{BMO}(\partial\Omega)$, *one has*

$$\mathrm{dist}(\nu, \mathrm{VMO}(\partial\Omega)) \leq 4\|\mathcal{C}^{\mathrm{pv}}\|_* \left(\sum_{j=1}^{n} \mathrm{dist}(R_j 1, \mathrm{VMO}(\partial\Omega))^2 \right)^{\frac{1}{2}}, \tag{7-15}$$

$$\left(\sum_{j=1}^{n} \mathrm{dist}(R_j 1, \mathrm{VMO}(\partial\Omega))^2 \right)^{\frac{1}{2}} \leq \|\mathcal{C}^{\mathrm{pv}}\|_* \,\mathrm{dist}(\nu, \mathrm{VMO}(\partial\Omega)). \tag{7-16}$$

Proof. On the one hand, based on (6-50), Proposition 7.1 and the fact that each $R_j^{\rm pv}$ agrees with R_j on $L^2(\partial\Omega)$, we may estimate

$$\begin{aligned}
\operatorname{dist}(\nu, \mathrm{VMO}(\partial\Omega)) &= \inf_{\eta\in\mathrm{VMO}(\partial\Omega)} [\nu-\eta]_{\mathrm{BMO}(\partial\Omega)} \\
&= \inf_{\eta\in\mathrm{VMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} [\nu-\eta]_{\mathrm{BMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} \\
&= \inf_{\eta\in\mathrm{VMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} 4\Big[\mathcal{C}^{\rm pv}\Big(\sum_{j=1}^n (R_j^{\rm pv}1)e_j+\mathcal{C}^{\rm pv}\eta\Big)\Big]_{\mathrm{BMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} \\
&\le 4\|\mathcal{C}^{\rm pv}\|_* \inf_{\eta\in\mathrm{VMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} \Big[\sum_{j=1}^n (R_j1)e_j+\mathcal{C}^{\rm pv}\eta\Big]_{\mathrm{BMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} \\
&= 4\|\mathcal{C}^{\rm pv}\|_* \inf_{\xi\in\mathrm{VMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} \Big[\sum_{j=1}^n (R_j1)e_j-\xi\Big]_{\mathrm{BMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} \\
&= 4\|\mathcal{C}^{\rm pv}\|_* \inf_{\xi\in\mathrm{VMO}(\partial\Omega)} \Big[\sum_{j=1}^n (R_j1)e_j-\xi\Big]_{\mathrm{BMO}(\partial\Omega)} \\
&= 4\|\mathcal{C}^{\rm pv}\|_* \Big(\sum_{j=1}^n \operatorname{dist}(R_j1, \mathrm{VMO}(\partial\Omega))^2\Big)^{\frac12},
\end{aligned}\tag{7-17}$$

yielding (7-15). On the other hand, from (6-49) and Proposition 7.1 we deduce — once again by bearing in mind that each $R_j^{\rm pv}$ agrees with R_j on $L^2(\partial\Omega)$ — that

$$\begin{aligned}
\Big(\sum_{j=1}^n \operatorname{dist}(R_j1, \mathrm{VMO}(\partial\Omega))^2\Big)^{\frac12} &= \inf_{\xi\in\mathrm{VMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} \Big[\sum_{j=1}^n (R_j1)e_j-\xi\Big]_{\mathrm{BMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} \\
&= \inf_{\xi\in\mathrm{VMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} \Big[\sum_{j=1}^n (R_j^{\rm pv}1)e_j-\xi\Big]_{\mathrm{BMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} \\
&= \inf_{\xi\in\mathrm{VMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} [\mathcal{C}^{\rm pv}\nu-\xi]_{\mathrm{BMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} \\
&= \inf_{\eta\in\mathrm{VMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} [\mathcal{C}^{\rm pv}(\nu-\eta)]_{\mathrm{BMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} \\
&\le \|\mathcal{C}^{\rm pv}\|_* \inf_{\eta\in\mathrm{VMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} [\nu-\eta]_{\mathrm{BMO}(\partial\Omega)\otimes\mathcal{C}\ell_n} \\
&= \|\mathcal{C}^{\rm pv}\|_* \inf_{\eta\in\mathrm{VMO}(\partial\Omega)} [\nu-\eta]_{\mathrm{BMO}(\partial\Omega)} \\
&= \|\mathcal{C}^{\rm pv}\|_* \operatorname{dist}(\nu, \mathrm{VMO}(\partial\Omega)),
\end{aligned}\tag{7-18}$$

finishing the justification of (7-16). □

Having established Theorem 7.2, we are now in a position to present the proof of Theorem 1.4.

Proof of Theorem 1.4. For the left-to-right implication in (1-28), first observe that Ω is a UR domain (see Definition 2.7). As such, Theorem 7.2 applies and (7-16) gives $R_j1 \in \mathrm{VMO}(\partial\Omega)$ for each $j \in \{1, \dots, n\}$.

For the right-to-left implication in (1-28), use (1-11) and the background assumptions on Ω to conclude that Ω is a UR domain, then invoke (7-15) from Theorem 7.2 to conclude that $\nu \in \mathrm{VMO}(\partial\Omega)$. □

Moving on, we record the following definition:

Definition 7.3. Let $\Omega \subset \mathbb{R}^n$ be an open set with compact boundary. Then Ω is said to satisfy a *John condition* if there exist $\theta \in (0, 1)$ and $R \in (0, \infty)$, called the John constants of Ω, with the following significance: for every $p \in \partial\Omega$ and $r \in (0, R)$ one can find $p_r \in B(p, r) \cap \Omega$ such that $B(p_r, \theta r) \subset \Omega$ and with the property that, for each $x \in B(p, r) \cap \partial\Omega$, there exists a rectifiable path $\gamma_x : [0, 1] \to \overline{\Omega}$ whose length is at most $\theta^{-1} r$ and

$$\gamma_x(0) = x, \quad \gamma_x(1) = p_r \quad \text{and} \quad \operatorname{dist}(\gamma_x(t), \partial\Omega) > \theta|\gamma_x(t) - x| \quad \text{for all } t \in (0, 1]. \tag{7-19}$$

Furthermore, Ω is said to satisfy a *two-sided John condition* if both Ω and $\mathbb{R}^n \setminus \overline{\Omega}$ satisfy a John condition.

The above definition appears in [Hofmann et al. 2010], where it was noted that any NTA domain (in the sense of D. Jerison and C. Kenig [1982]) with compact boundary satisfies a John condition.

Next, we recall the concept of δ-Reifenberg flat domain, following [Kenig and Toro 1999; 2003]. As a preamble, the reader is reminded that the Pompeiu–Hausdorff distance between two sets $A, B \subseteq \mathbb{R}^n$ is given by

$$D[A, B] := \max\bigl\{\sup\{\operatorname{dist}(a, B) : a \in A\},\ \sup\{\operatorname{dist}(b, A) : b \in B\}\bigr\}. \tag{7-20}$$

Definition 7.4. Let $\Sigma \subset \mathbb{R}^n$ be a compact set and let $\delta \in (0, 1/(4\sqrt{2}))$. Call Σ a *δ-Reifenberg flat set* if there exists $R > 0$ such that, for every $x \in \Sigma$ and every $r \in (0, R]$, there exists an $(n-1)$-dimensional plane $L(x, r)$ which contains x and is such that

$$D[\Sigma \cap B(x, r), L(x, r) \cap B(x, r)] \le \delta r. \tag{7-21}$$

Definition 7.5. Say that a bounded open set $\Omega \subset \mathbb{R}^n$ has the *separation property* if there exists $R > 0$ such that, for every $x \in \partial\Omega$ and $r \in (0, R]$, there exists an $(n-1)$-dimensional plane $\mathcal{L}(x, r)$ containing x and a choice of unit normal vector to $\mathcal{L}(x, r)$ — call it $\vec{n}_{x,r}$ — satisfying

$$\begin{aligned} &\bigl\{y + t\vec{n}_{x,r} \in B(x, r) : y \in \mathcal{L}(x, r),\ t < -\tfrac{1}{4}r\bigr\} \subset \Omega, \\ &\bigl\{y + t\,\vec{n}_{x,r} \in B(x, r) : y \in \mathcal{L}(x, r),\ t > \tfrac{1}{4}r\bigr\} \subset \mathbb{R}^n \setminus \Omega. \end{aligned} \tag{7-22}$$

Moreover, if Ω is unbounded, it is also required that $\partial\Omega$ divides $\mathbb{R}^n$ into two distinct connected components and that $\mathbb{R}^n \setminus \Omega$ has a nonempty interior.

Definition 7.6. Let $\Omega \subset \mathbb{R}^n$ be a bounded open set and $\delta \in (0, \delta_n)$. Call Ω a *δ-Reifenberg flat domain* if Ω has the separation property and $\partial\Omega$ is a δ-Reifenberg flat set.

The notion of *Reifenberg flat domain with vanishing constant* is introduced in a similar fashion, this time allowing the constant δ appearing in (7-21) to depend on r, say $\delta = \delta(r)$, and demanding that $\lim_{r\to 0^+} \delta(r) = 0$.

As our next result shows, under appropriate background assumptions (of a "large" geometry nature) the proximity of the vector-valued function $(R_1 1, R_2 1, \dots, R_n 1)$ to the space $\mathrm{VMO}(\partial\Omega)$, measured in $\mathrm{BMO}(\partial\Omega)$, can be used to quantify Reifenberg flatness.

Theorem 7.7. *Assume $\Omega \subseteq \mathbb{R}^n$ is an open set with a compact Ahlfors regular boundary, satisfying a two-sided John condition* (hence, Ω is a UR domain, which further entails that $R_j 1 \in \mathrm{BMO}(\partial\Omega)$ for each j). *If, with distances considered in* $\mathrm{BMO}(\partial\Omega)$,

$$\sum_{j=1}^{n} \mathrm{dist}(R_j 1, \mathrm{VMO}(\partial\Omega)) < \varepsilon, \tag{7-23}$$

then Ω is a δ-Reifenberg flat domain for $\delta = C_o \cdot \varepsilon$, where $C_o \in (0, \infty)$ depends only on the Ahlfors regularity and John constants of Ω.

As a consequence, if $R_j 1 \in \mathrm{VMO}(\partial\Omega)$ for every $j \in \{1, \dots, n\}$ then actually Ω is a Reifenberg flat domain with vanishing constant.

Proof. It is known that if $\Omega \subseteq \mathbb{R}^n$ is an open set with a compact Ahlfors regular boundary, satisfying a two-sided John condition, and such that

$$\mathrm{dist}(\nu, \mathrm{VMO}(\partial\Omega)) < \varepsilon \tag{7-24}$$

(with the distance considered in $\mathrm{BMO}(\partial\Omega)$), then Ω is a δ-Reifenberg flat domain for the choice $\delta = C_o \cdot \varepsilon$, where the constant $C_o \in (0, \infty)$ is as in the statement of the theorem. See [Hofmann et al. 2010, Definition 4.7, p. 2690 and Corollary 4.20, p. 2710] in this regard. Granted this, the desired conclusion follows by invoking Theorem 7.2, since our assumptions on Ω guarantee that this is a UR domain (see (1-29)). □

In this last part of this section we discuss a (partial) extension of Theorem 1.1 in the context of Besov spaces. We begin by defining this scale and recalling some of its most basic properties.

Definition 7.8. Assume that $\Sigma \subset \mathbb{R}^n$ is an Ahlfors regular set and let $\sigma := \mathcal{H}^{n-1} \lfloor \Sigma$. Then, given $1 \le p \le \infty$ and $0 < s < 1$, define the Besov space

$$B_s^{p,p}(\Sigma) := \{f \in L^p(\Sigma, \sigma) : \|f\|_{B_s^{p,p}(\Sigma)} < +\infty\}, \tag{7-25}$$

where

$$\|f\|_{B_s^{p,p}(\Sigma)} := \|f\|_{L^p(\Sigma,\sigma)} + \left(\int_\Sigma \int_\Sigma \frac{|f(x) - f(y)|^p}{|x-y|^{n-1+sp}}\, d\sigma(x)\, d\sigma(y)\right)^{\frac{1}{p}}, \tag{7-26}$$

with the convention that

$$B_s^{\infty,\infty}(\Sigma) := \mathscr{C}^s(\Sigma) \quad \text{and} \quad \|f\|_{B_s^{\infty,\infty}(\Sigma)} := \|f\|_{\mathscr{C}^s(\Sigma)}. \tag{7-27}$$

Finally, denote by $B_{s,\,\mathrm{loc}}^{p,p}(\Sigma)$ the space of functions whose truncations by smooth and compactly supported functions belong to $B_s^{p,p}(\Sigma)$.

Consider Σ as in Definition 7.8 and suppose $1 \le p_0, p_1 \le \infty$ and $s_0, s_1 \in (0, 1)$ are such that

$$\frac{1}{p_1} - \frac{s_1}{n-1} = \frac{1}{p_0} - \frac{s_0}{n-1} \quad \text{and} \quad s_0 \ge s_1. \tag{7-28}$$

Then [Jonsson and Wallin 1984, Proposition 5, p. 213] gives that

$$B^{p_0,p_0}_{s_0}(\Sigma) \hookrightarrow B^{p_1,p_1}_{s_1}(\Sigma) \quad \text{continuously.} \tag{7-29}$$

In particular,

$$B^{p,p}_s(\Sigma) \hookrightarrow \mathscr{C}^\alpha(\Sigma) \quad \text{if } p \in [1,\infty],\ s \in (0,1) \text{ with } sp > n-1,\ \alpha := s - \frac{n-1}{p}. \tag{7-30}$$

In turn, from (7-25)–(7-26) and (7-30) one may easily deduce that

$$B^{p,p}_s(\Sigma) \text{ is an algebra if } p \in [1,\infty] \text{ and } s \in (0,1) \text{ satisfy } sp > n-1, \tag{7-31}$$

and

$$f/g \in B^{p,p}_s(\Sigma) \text{ whenever } f, g \in B^{p,p}_s(\Sigma) \text{ and } |g| \geq c > 0\ \sigma\text{-a.e. on } \Sigma. \tag{7-32}$$

Another useful simple property is that, given any $p \in [1,\infty]$ and $s \in (0,1)$, if $F : \mathbb{R} \to \mathbb{R}$ is a bounded Lipschitz function then

$$F \circ f \in B^{p,p}_{s,\mathrm{loc}}(\Sigma) \quad \text{for every } f \in B^{p,p}_s(\Sigma). \tag{7-33}$$

Finally, we note that in the case when Σ is the graph of a Lipschitz function $\varphi : \mathbb{R}^{n-1} \to \mathbb{R}$, from [Mitrea and Mitrea 2013, Proposition 2.9, p. 33] and real interpolation we obtain that, for each $p \in (1,\infty)$ and $s \in (0,1)$,

$$f \in B^{p,p}_s(\Sigma) \iff f(\cdot, \varphi(\cdot)) \in B^{p,p}_s(\mathbb{R}^{n-1}). \tag{7-34}$$

Proposition 7.9. *Assume $\Omega \subset \mathbb{R}^n$ is a Lebesgue measurable set whose boundary is compact, Ahlfors regular, and satisfies* (2-16). *Then*

$$\mathcal{C}^{\mathrm{pv}} : B^{p,p}_s(\partial\Omega) \otimes \mathcal{C}\ell_n \longrightarrow B^{p,p}_s(\partial\Omega) \otimes \mathcal{C}\ell_n \tag{7-35}$$

is well-defined and bounded for each $p \in [1,\infty]$ and $s \in (0,1)$.

Proof. One way to see this is via real interpolation (see [Han et al. 2008, §8.1] for a version suiting the current setting) between the boundedness result proved in Theorem 5.6 (corresponding to (7-35) when $p = \infty$; see (7-27)), and the fact that the operator $\mathcal{C}^{\mathrm{pv}}$ in (7-35) with $p = 1$ is also bounded (which follows from the atomic/molecular theory for the Besov scale on spaces of homogeneous type from [Han and Yang 2003]). ☐

In order to present the extension of Theorem 1.1 mentioned earlier to the scale of Besov spaces, we make the following definition:

Definition 7.10. Given $p \in [1,\infty]$ and $s \in (0,1)$, call a nonempty, open, proper subset Ω of $\mathbb{R}^n$ a $B^{p,p}_{s+1}$*-domain* provided it may be locally identified[5] near boundary points with the upper graph of a real-valued function φ defined in $\mathbb{R}^{n-1}$ with the property that $\partial_j\varphi \in B^{p,p}_s(\mathbb{R}^{n-1})$ for each $j \in \{1,\dots,n-1\}$.

The stage has been set for stating and proving the following result:

[5]In the sense described in Definition 2.1.

Theorem 7.11. *Assume $\Omega \subseteq \mathbb{R}^n$ is an Ahlfors regular domain with a compact boundary, satisfying $\partial\Omega = \partial(\overline{\Omega})$. Then, for each $s \in (0, 1)$ and $p \in [1, \infty]$ with the property that $sp > n - 1$, the following claims are equivalent*:

(a) *Ω is a $B^{p,p}_{s+1}$ domain.*

(b) *The distributional Riesz transforms associated with $\partial\Omega$ satisfy*

$$R_j 1 \in B^{p,p}_s(\partial\Omega) \quad \textit{for each } j \in \{1, \dots, n\}. \tag{7-36}$$

Proof. Consider the implication (b) $\Longrightarrow$ (a). The starting point is the observation that (7-36) and (7-30) imply (1-14) for $\alpha := s - (n-1)/p \in (0, 1)$. As such, Theorem 1.1 applies and gives that Ω is a domain of class $\mathscr{C}^{1+\alpha}$. Hence, locally, the outward unit normal ν to Ω has components $(\nu_j)_{1 \le j \le n}$ of the form

$$\nu_j(x', \varphi(x')) = \begin{cases} \dfrac{\partial_j \varphi(x')}{\sqrt{1 + |\nabla\varphi(x')|^2}} & \text{if } 1 \le j \le n-1, \\ -\dfrac{1}{\sqrt{1+|\nabla\varphi(x')|^2}} & \text{if } j = n, \end{cases} \tag{7-37}$$

where $\varphi \in \mathscr{C}^{1+\alpha}(\mathbb{R}^{n-1})$ is a real-valued function whose upper graph locally describes Ω. Without loss of generality it may be assumed that φ has compact support.

On the other hand, from the assumption (7-36), Proposition 7.9 and (6-50) we may conclude that

$$\nu \in B^{p,p}_s(\partial\Omega). \tag{7-38}$$

On account of this membership and (7-34), we obtain

$$\nu_j(\cdot, \varphi(\cdot)) \in B^{p,p}_s(\mathbb{R}^{n-1}) \quad \text{for each } j \in \{1, \dots, n\}. \tag{7-39}$$

Upon recalling (7-31)–(7-32), this further yields

$$\partial_j \varphi = \frac{\nu_j(\cdot, \varphi(\cdot))}{\nu_n(\cdot, \varphi(\cdot))} \in B^{p,p}_s(\mathbb{R}^{n-1}) \quad \text{for each } j \in \{1, \dots, n-1\}, \tag{7-40}$$

proving that Ω is a $B^{p,p}_{s+1}$ domain.

Concerning the implication (a) $\Longrightarrow$ (b), assume that Ω is a $B^{p,p}_{s+1}$ domain with s and p as before. From the definitions and (7-30) (used with $\Sigma := \mathbb{R}^{n-1}$) it follows that Ω is a domain of class $\mathscr{C}^{1+\alpha}$ with $\alpha := s - (n-1)/p$. Hence, in particular, Ω is a Lipschitz domain. We claim that (7-38) holds. Thanks to (7-34), justifying this claim comes down to proving that (7-39) holds, where φ is a real-valued function defined in $\mathbb{R}^{n-1}$ satisfying $\partial_j \varphi \in B^{p,p}_s(\mathbb{R}^{n-1})$ for each $j \in \{1, \dots, n-1\}$ and whose upper graph locally describes Ω (again, without loss of generality it may be assumed that φ has compact support). To this end, consider the function $F : \mathbb{R} \to \mathbb{R}$ given by $F(t) := 1/\sqrt{1 + |t|}$ for each $t \in \mathbb{R}$, and note that F is both bounded and Lipschitz. Since, by (7-31),

$$|\nabla\varphi|^2 = \sum_{j=1}^{n-1} (\partial_j \varphi)(\partial_j \varphi) \in B^{p,p}_s(\mathbb{R}^{n-1}), \tag{7-41}$$

it follows from (7-33) that

$$\nu_n(\,\cdot\,,\varphi(\,\cdot\,)) = -F \circ |\nabla\varphi|^2 \in B^{p,p}_{s,\mathrm{loc}}(\mathbb{R}^{n-1}). \tag{7-42}$$

Granted this, another reference to (7-31) gives that, for each $j \in \{1,\dots,n-1\}$,

$$\nu_j(\,\cdot\,,\varphi(\,\cdot\,)) = \frac{\partial_j\varphi}{\sqrt{1+|\nabla\varphi|^2}} = -\partial_j\varphi\cdot\nu_n(\,\cdot\,,\varphi(\,\cdot\,)) \in B^{p,p}_s(\mathbb{R}^{n-1}). \tag{7-43}$$

This finishes the proof of (7-39), hence completing the justification of (7-38). Having established this, bring in identity (6-49) in order to conclude, on account of Proposition 7.9, that

$$\sum_{j=1}^{n}(R_j 1)e_j = \sum_{j=1}^{n}(R_j^{\mathrm{pv}} 1)e_j = -\mathcal{C}^{\mathrm{pv}}\nu \in B^{p,p}_s(\partial\Omega)\otimes\mathcal{C}\ell_n. \tag{7-44}$$

Since this readily implies (7-36), the implication (a) $\Longrightarrow$ (b) is established. □

Lastly, we remark that the limiting case $s = 1$ of Theorem 7.11 also holds provided $p \in (n-1,\infty)$ and the Besov space intervening in (7-36) is replaced by $L^p_1(\partial\Omega)$, the L^p-based Sobolev space of order 1 on $\partial\Omega$ considered in [Hofmann et al. 2010] (in which scenario Ω is an L^p_2 domain, in a natural sense). The proof follows the same blueprint and makes use of the fact that $\mathcal{C}^{\mathrm{pv}}$ is a bounded operator from $L^p_1(\partial\Omega)\otimes\mathcal{C}\ell_n$ into itself (see [Mitrea et al. 2015; 2016] in this regard).

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References

[Alexander 1978] S. Alexander, "Local and global convexity in complete Riemannian manifolds", *Pacific J. Math.* **76**:2 (1978), 283–289. MR 506131 Zbl 0384.52003

[Alvarado and Mitrea 2015] R. Alvarado and M. Mitrea, *Hardy spaces on Ahlfors-regular quasi metric spaces: a sharp theory*, Lecture Notes in Mathematics **2142**, Springer, Cham, 2015. MR 3310009 Zbl 1322.30001

[Alvarado et al. 2011] R. Alvarado, D. Brigham, V. Maz'ya, M. Mitrea, and E. Ziadé, "On the regularity of domains satisfying a uniform hour-glass condition and a sharp version of the Hopf–Oleinik boundary point principle", *Probl. Mat. Anal.* **57** (2011), 3–68. In Russian; translated in *J. Math. Sci. (N. Y.)* **176**:3 (2011), 281–360. MR 2839047 Zbl 1290.35046

[Auscher and Hytönen 2013] P. Auscher and T. Hytönen, "Orthonormal bases of regular wavelets in spaces of homogeneous type", *Appl. Comput. Harmon. Anal.* **34**:2 (2013), 266–296. MR 3008566 Zbl 1261.42057

[Brackx et al. 1982] F. Brackx, R. Delanghe, and F. Sommen, *Clifford analysis*, Research Notes in Mathematics **76**, Pitman, Boston, 1982. MR 697564 Zbl 0529.30001

[Christ 1990] M. Christ, *Lectures on singular integral operators*, CBMS Regional Conference Series in Mathematics **77**, American Mathematical Society, Providence, RI, 1990. MR 1104656 Zbl 0745.42008

[Coifman and Weiss 1971] R. R. Coifman and G. Weiss, *Analyse harmonique non-commutative sur certains espaces homogènes: étude de certaines intégrales singulières*, Lecture Notes in Mathematics **242**, Springer, Berlin, 1971. MR 0499948 Zbl 0224.43006

[Coifman and Weiss 1977] R. R. Coifman and G. Weiss, "Extensions of Hardy spaces and their use in analysis", *Bull. Amer. Math. Soc.* **83**:4 (1977), 569–645. MR 0447954 Zbl 0358.30023

[Colton and Kress 1983] D. L. Colton and R. Kress, *Integral equation methods in scattering theory*, John Wiley & Sons, New York, 1983. MR 700400 Zbl 0522.35001

[David 1991] G. David, *Wavelets and singular integrals on curves and surfaces*, Lecture Notes in Mathematics **1465**, Springer, Berlin, 1991. MR 1123480 Zbl 0764.42019

[David and Journé 1984] G. David and J.-L. Journé, "A boundedness criterion for generalized Calderón–Zygmund operators", *Ann. of Math.* (2) **120**:2 (1984), 371–397. MR 763911 Zbl 0567.47025

[David and Semmes 1991] G. David and S. Semmes, *Singular integrals and rectifiable sets in* $\mathbf{R}^n$*: beyond Lipschitz graphs*, Astérisque **193**, 1991. MR 1113517 Zbl 0743.49018

[David and Semmes 1993] G. David and S. Semmes, *Analysis of and on uniformly rectifiable sets*, Mathematical Surveys and Monographs **38**, American Mathematical Society, Providence, RI, 1993. MR 1251061 Zbl 0832.42008

[Dyn′kin 1979] E. M. Dyn′kin, "Smoothness of Cauchy type integrals", *Zap. Nauchn. Sem. Leningrad. Otdel. Mat. Inst. Steklov.* (*LOMI*) **92** (1979), 115–133, 320–321. In Russian. MR 566745 Zbl 0432.30033

[Dyn′kin 1980] E. M. Dyn′kin, "Smoothness of Cauchy type integrals", *Dokl. Akad. Nauk SSSR* **250**:4 (1980), 794–797. In Russian; translated in *Sov. Math., Dokl.* **21** (1980), 199–202. MR 560377

[Evans and Gariepy 1992] L. C. Evans and R. F. Gariepy, *Measure theory and fine properties of functions*, CRC Press, Boca Raton, FL, 1992. MR 1158660 Zbl 0804.28001

[Fabes et al. 1999] E. Fabes, I. Mitrea, and M. Mitrea, "On the boundedness of singular integrals", *Pacific J. Math.* **189**:1 (1999), 21–29. MR 1687806 Zbl 1054.42503

[Federer 1969] H. Federer, *Geometric measure theory*, Grundlehren der Math. Wissenschaften **153**, Springer, New York, 1969. MR 0257325 Zbl 0176.00801

[Gakhov 1966] F. D. Gakhov, *Boundary value problems*, edited by I. N. Sneddon, Pergamon Press, Oxford, 1966. MR 0198152 Zbl 0141.08001

[García-Cuerva and Gatto 2005] J. García-Cuerva and A. E. Gatto, "Lipschitz spaces and Calderón–Zygmund operators associated to non-doubling measures", *Publ. Mat.* **49**:2 (2005), 285–296. MR 2177069 Zbl 1077.42011

[Gatto 2009] A. E. Gatto, "Boundedness on inhomogeneous Lipschitz spaces of fractional integrals singular integrals and hypersingular integrals associated to non-doubling measures", *Collect. Math.* **60**:1 (2009), 101–114. MR 2490753 Zbl 1196.42013

[Han and Yang 2003] Y. Han and D. Yang, "Some new spaces of Besov and Triebel–Lizorkin type on homogeneous spaces", *Studia Math.* **156**:1 (2003), 67–97. MR 1961062 Zbl 1032.42025

[Han et al. 2008] Y. Han, D. Müller, and D. Yang, "A theory of Besov and Triebel–Lizorkin spaces on metric measure spaces modeled on Carnot-Carathéodory spaces", *Abstr. Appl. Anal.* **2008** (2008), art. ID 893409. MR 2485404 Zbl 1193.46018

[Hofmann et al. 2007] S. Hofmann, M. Mitrea, and M. Taylor, "Geometric and transformational properties of Lipschitz domains, Semmes–Kenig–Toro domains, and other classes of finite perimeter domains", *J. Geom. Anal.* **17**:4 (2007), 593–647. MR 2365661 Zbl 1142.49021

[Hofmann et al. 2010] S. Hofmann, M. Mitrea, and M. Taylor, "Singular integrals and elliptic boundary problems on regular Semmes–Kenig–Toro domains", *Int. Math. Res. Not.* **2010**:14 (2010), 2567–2865. MR 2669659

[Hofmann et al. 2015] S. Hofmann, M. Mitrea, and M. E. Taylor, "Symbol calculus for operators of layer potential type on Lipschitz surfaces with VMO normals, and related pseudodifferential operator calculus", *Anal. PDE* **8**:1 (2015), 115–181. MR 3336923 Zbl 1317.31012

[Hsiao and Wendland 2008] G. C. Hsiao and W. L. Wendland, *Boundary integral equations*, Applied Mathematical Sciences **164**, Springer, Berlin, 2008. MR 2441884 Zbl 1157.65066

[Iftimie 1965] V. Iftimie, "Fonctions hypercomplexes", *Bull. Math. Soc. Sci. Math. R. S. Roumanie* **9** (1965), 279–332. MR 0217312 Zbl 0177.36903

[Jerison and Kenig 1982] D. S. Jerison and C. E. Kenig, "Boundary behavior of harmonic functions in nontangentially accessible domains", *Adv. in Math.* **46**:1 (1982), 80–147. MR 676988 Zbl 0514.31003

[Jonsson and Wallin 1984] A. Jonsson and H. Wallin, *Function spaces on subsets of* $\mathbf{R}^n$, Math. Rep. **1**, 1984. MR 820626 Zbl 0875.46003

[Kenig and Toro 1999] C. E. Kenig and T. Toro, "Free boundary regularity for harmonic measures and Poisson kernels", *Ann. of Math.* (2) **150**:2 (1999), 369–454. MR 1726699 Zbl 0946.31001

[Kenig and Toro 2003] C. E. Kenig and T. Toro, "Poisson kernel characterization of Reifenberg flat chord arc domains", *Ann. Sci. École Norm. Sup.* (4) **36**:3 (2003), 323–401. MR 1977823 Zbl 1027.31005

[Kress 1989] R. Kress, *Linear integral equations*, Applied Mathematical Sciences **82**, Springer, Berlin, 1989. MR 1007594 Zbl 0671.45001

[Martio and Sarvas 1979] O. Martio and J. Sarvas, "Injectivity theorems in plane and space", *Ann. Acad. Sci. Fenn. Ser. A I Math.* **4**:2 (1979), 383–401. MR 565886 Zbl 0406.30013

[Mateu et al. 2009] J. Mateu, J. Orobitg, and J. Verdera, "Extra cancellation of even Calderón–Zygmund operators and quasiconformal mappings", *J. Math. Pures Appl.* (9) **91**:4 (2009), 402–431. MR 2518005 Zbl 1179.30017

[Mattila et al. 1996] P. Mattila, M. S. Melnikov, and J. Verdera, "The Cauchy integral, analytic capacity, and uniform rectifiability", *Ann. of Math.* (2) **144**:1 (1996), 127–136. MR 1405945 Zbl 0897.42007

[Meyer 1990] Y. Meyer, *Ondelettes et opérateurs, II: Opérateurs de Calderón–Zygmund*, Hermann, Paris, 1990. MR 1085488

[Mitrea 1994] M. Mitrea, *Clifford wavelets, singular integrals, and Hardy spaces*, Lecture Notes in Mathematics **1575**, Springer, Berlin, 1994. MR 1295843 Zbl 0822.42018

[Mitrea 2013] D. Mitrea, *Distributions, partial differential equations, and harmonic analysis*, Springer, New York, 2013. MR 3114783 Zbl 1308.46002

[Mitrea and Mitrea 2013] I. Mitrea and M. Mitrea, *Multi-layer potentials and boundary problems for higher-order elliptic systems in Lipschitz domains*, Lecture Notes in Mathematics **2063**, Springer, Heidelberg, 2013. MR 3013645 Zbl 1268.35001

[Mitrea et al. 2015] I. Mitrea, M. Mitrea, and M. Taylor, "Cauchy integrals, Calderón projectors, and Toeplitz operators on uniformly rectifiable domains", *Adv. Math.* **268** (2015), 666–757. MR 3276607 Zbl 1305.31003

[Mitrea et al. 2016] I. Mitrea, M. Mitrea, and M. Taylor, "Riemann–Hilbert problems, Cauchy integrals, and Toeplitz operators on uniformly rectifiable domains", book manuscript, 2016.

[Muskhelishvili 1953] N. I. Muskhelishvili, *Singular integral equations: boundary problems of function theory and their application to mathematical physics*, Noordhoff, Groningen, 1953. MR 1215485 Zbl 0051.33203

[Nazarov et al. 2014] F. Nazarov, X. Tolsa, and A. Volberg, "On the uniform rectifiability of AD-regular measures with bounded Riesz transform operator: the case of codimension 1", *Acta Math.* **213**:2 (2014), 237–321. MR 3286036 Zbl 1311.28004

[Plemelj 1908] J. Plemelj, "Ein Ergänzungssatz zur Cauchyschen Integraldarstellung analytischer Funktionen, Randwerte betreffend", *Monatsh. Math. Phys.* **19**:1 (1908), 205–210. MR 1547763 Zbl 39.0460.01

[Privalov 1918] I. I. Privalov, *The Cauchy integral*, Saratov, 1918. In Russian.

[Privalov 1941] I. I. Privalov, *Limiting properties of single-valued analytic functions*, Publ. Moscow State University, 1941.

[Semmes 1989] S. W. Semmes, "A criterion for the boundedness of singular integrals on hypersurfaces", *Trans. Amer. Math. Soc.* **311**:2 (1989), 501–513. MR 948198 Zbl 0675.42015

[Stein 1970] E. M. Stein, *Singular integrals and differentiability properties of functions*, Princeton Mathematical Series **30**, Princeton University Press, Princeton, N.J., 1970. MR 0290095 Zbl 0207.13501

[Taylor 2000] M. E. Taylor, *Tools for PDE: pseudodifferential operators, paradifferential operators, and layer potentials*, Mathematical Surveys and Monographs **81**, American Mathematical Society, Providence, RI, 2000. MR 1766415 Zbl 0963.35211

[Tolsa 2008] X. Tolsa, "Principal values for Riesz transforms and rectifiability", *J. Funct. Anal.* **254**:7 (2008), 1811–1863. MR 2397876 Zbl 1153.28003

[Wittmann 1987] R. Wittmann, “Application of a theorem of M. G. Kreĭn to singular integrals”, *Trans. Amer. Math. Soc.* **299**:2 (1987), 581–599. MR 869223 Zbl 0596.42005

[Ziemer 1989] W. P. Ziemer, *Weakly differentiable functions: Sobolev spaces and functions of bounded variation*, Graduate Texts in Mathematics **120**, Springer, New York, 1989. MR 1014685 Zbl 0692.46022

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