PROPAGATION OF SINGULARITIES AND GROWTH FOR SCHRÖDINGER OPERATORS

JARED WUNSCH

Abstract. We study the time-dependent Schrödinger equation $(D_t + \frac{1}{2}\Delta + V)\psi = 0$ for the Laplacian of a scattering metric on a compact manifold with boundary. Under a non-trapping hypothesis on the geodesics, the microlocal smoothness of $\psi(t)$ is determined by growth properties of $\psi(0)$ as measured by the "quadratic-scattering" wavefront set, a generalization of Hörmander's wavefront set. We prove a propagation theorem for the quadratic-scattering wavefront set which describes singularities and growth of $\psi(t, \cdot)$ in terms of singularities and growth of $\psi(0, \cdot)$.

Date: June 3, 1998.

Contents

1. Introduction 3
2. Geometric preliminaries 6
3. The scattering calculus 7
4. The quadratic-scattering calculus 10
5. Invariant definition of the quadratic-scattering calculus 11
6. Symbol maps 14
7. Quantization 19
8. Sobolev spaces 20
9. Wavefront sets 21
10. The Schrödinger equation 23
11. Bicharacteristic flow 25
12. The main theorems 32
13. Symbol construction 36
Construction of $\mathfrak{a}_\partial$ 37
Construction of $\mathfrak{a}_+$ and $\tilde{\mathfrak{a}}_+$ 38
Construction of $\mathfrak{a}_\circ$ and $\tilde{\mathfrak{a}}_\circ$ 39
Construction of $\mathfrak{a}_-$ and $\tilde{\mathfrak{a}}_-$ 40
14. Proof of the main theorems 41
Proof of Theorem 12.1 41
Proof of Theorem 12.2, part 1 44
Proof of Theorem 12.3, part 1 47
Proof of Theorem 12.4 47
Proof of Theorem 12.5 48
References 49

1. Introduction

The time-dependent Schrödinger equation is the non-relativistic quantum-mechanical description of the motion of a particle in a potential. In appropriate units, the equation reads

$$(D_t + \frac{1}{2}\Delta + V)\psi = 0 \tag{1.1}$$

where $D_t = -i\frac{\partial}{\partial t}$, Δ is the (non-negative) Laplace-Beltrami operator with respect to a Riemannian metric, and V can be a real multiplication operator or, by incorporating a "magnetic potential term," the sum of a multiplication operator and a first-order, self-adjoint differential operator. The standard interpretation of this equation is that $|\psi(t,z)|^2$ is the probability density of observing the particle at the point z at time t. For the sake of convenience, we write $\psi(t) = \psi(t,\cdot)$.

We are interested in the propagation of singularities for the Schrödinger equation. The regularity of solutions is already interesting on $\mathbb{R}^1$, with $V = 0$. In that case, the fundamental solution is given by

$$K_t(z,w) = (2\pi i t)^{-\frac{1}{2}} e^{i|z-w|^2/2t}. \tag{1.2}$$

Thus,

$$\psi(t,z) = \int K_t(z,w)\psi(0,w)dw = (2\pi i t)^{-\frac{1}{2}} e^{iz^2/2t}\mathcal{F}_w\left(e^{iw^2/2t}\psi(0,w)\right)\left(\frac{z}{t}\right) \tag{1.3}$$

where $\mathcal{F}_w f = \int f(w)e^{-iw\cdot\xi}dw$ denotes the Fourier transform in w. Equation (1.3) has the interesting consequence that if $\psi(0) \in \mathcal{E}'(\mathbb{R}^1)$ then $\psi(t) \in \mathcal{C}^\infty(\mathbb{R}^1)$ for all $t > 0$. Conversely, however, if we start with the smooth initial data $\psi(0) = e^{-i\lambda z^2/2}$, then $\psi(t)$ develops a delta-function singularity at $t = \lambda^{-1}$. These examples, while showing that singularities do not propagate in the conventional sense of Hörmander's theorem (see [8]), do suggest that singularities are produced by asymptotic properties of the Cauchy data at infinity.

We now list a few works generalizing the above observations; the reader is referred to Craig, Kappeler, and Strauss [4] for a more complete discussion of recent work on propagation of singularities for the Schrödinger equation.

The first work on the propagation of singularities for the Schrödinger equation with variable-coefficient second-order terms (i.e. on curved space) seems to be that of Lascar [14] and Boutet de Monvel [1], who prove that the singularities of a solution to (1.1), considered as a function on spacetime, must be a union of geodesics in space, with time fixed; in other words, singularities travel at infinite speed along geodesics. This statement provides no information, however, about the singularities of the solution at time t in terms of Cauchy data. It also yields no information about the singularities in the spatial variables of the restriction of the solution to a fixed time.

Kapitanski and Safarov [12] prove results more tailored to the Cauchy problem: in the case in which $\frac{1}{2}\Delta + V$ in (1.1) is a real, variable-coefficient operator on $\mathbb{R}^n$ that has constant coefficients outside a large ball, they show that the fundamental solution is smooth for $t > 0$ under the assumption that there are no trapped bicharacteristics. Craig, Kappeler, and Strauss [4] allow operators in which the coefficients of the second-order term are asymptotically constant, and obtain conditions on the moments of $\psi(0)$ ensuring the *microlocal* smoothness of $\psi(t)$ at a given point for all $t > 0$. Conversely, a result on the *absence* of dispersive smoothing effects when the metric has trapped geodesics can be found in Doi [5].

The results of Kapitanski-Safarov and Craig-Kappeler-Strauss give smoothness for all $t > 0$ under appropriate hypotheses. On the other hand, in the case of the Euclidian metric, regularity results involving more interesting time-dependence have long been known. In [30], Zelditch obtains time-dependent information on the singularities of solutions to the harmonic-oscillator Schrödinger equation with a potential perturbation; he shows that the singularities "reconstruct" periodically. He also proves global, time-independent results on the regularity of the perturbed free-particle. Weinstein, in a related paper [28], proposes the introduction of a generalization of the wavefront set that measures behavior at infinity, and hence propagates well under time-evolution for the Schrödinger equation. He introduces a candidate for this set, the metawavefront set, and shows that if $p(x, \xi)$ is a real-valued polynomial of degree $\leqslant 2$ then for Hamiltonians on $\mathbb{R}^n$ that are perturbations of $p(x, D)$, the metawavefront set propagates nicely. Unfortunately, the metawavefront set is not in general closed, and its absence does not imply that a distribution is a Schwartz function.

Results on the harmonic-oscillator generalizing those of Zelditch to a broader class of potential perturbations have been recently obtained by Kapitanski, Rodnianski, and Yajima [11]. Another recent time-dependent result is that of Shananin [23], who proves a microlocal regularity result for the free, constant-coefficient Schrödinger equation with initial data of the form $a(z)e^{i\phi(z)}$.

Very strong tools are available in the Euclidian case which have not hitherto been developed in the general case: parametrices for $D_t - \frac{1}{2}\sum \partial_{z_i}^2 + V$ have been constructed by Treves [27] and Fujiwara [7]. Yajima [29] also uses a parametrix to obtain global regularity results in the Euclidian case; in addition, he demonstrates *lack* of regularity of the fundamental solution in the case of super-quadratic potentials.

In this paper, we generalize techniques used in [4] to prove time-dependent microlocal regularity results for a Schrödinger operator with potential terms on a Riemannian manifold. We follow the program of Weinstein [28], insofar as the results take the form of a propagation theorem for a generalized wavefront set which includes information about both growth and regularity. This wavefront set, which we call the "quadratic-scattering" (or "qsc") wavefront set, is closely related to the "scattering" wavefront set defined by Melrose in [15]. In the case of $\mathbb{R}^n$, the qsc wavefront set can be thought of as a subset of the boundary of the manifold with corners $B^n_z \times B^n_\xi$ (where B^n is the n-dimensional ball). We think of the first factor as the radial compactification of $\mathbb{R}^n_z$ and the second as a compactification of (a rescaled version of) $(\mathbb{R}^n_z)^*$. The boundary of $B^n_z \times B^n_\xi$ is composed of two faces: $\partial B^n_z \times B^n_\xi$, and $B^n_z \times \partial B^n_\xi$. The qsc wavefront set living in $(B^n_z)^\circ \times \partial B^n_\xi$ will be the ordinary wavefront set; the qsc wavefront set in $\partial B^n_z \times (B^n_\xi)^\circ$ is a measure of "quadratic oscillation at infinity." The wavefront set in the corner, $\partial B^n \times \partial B^n$, interpolates between the two notions in a sensible way. We let $\mathrm{WF}_{\mathrm{qsc}} u$ denote the qsc wavefront set of a distribution u.

We now describe the results of this paper in the case of $\mathbb{R}^n$ endowed with a "scattering" metric (this class of metrics includes asymptotically Euclidean metrics) and a potential term V that does not grow at infinity in a sense made precise in §10 (classical symbols of order zero, for example, are acceptable; harmonic oscillator potentials are not). Let ψ be a solution to (1.1). Given any point $p \in \partial(B^n_z \times B^n_\xi)$ and time $T > 0$, there is a set $\mathcal{G}_T(p) \subset \partial B^n_z \times (B^n_\xi)^\circ$ such that if $\mathrm{WF}_{\mathrm{qsc}}\psi(0) \cap \mathcal{G}_T(p) = \emptyset$ then $p \notin \mathrm{WF}_{\mathrm{qsc}}\psi(T)$. (The converse also holds if we assume uniformity in T; see §12 for details.)

On $\partial B^n_z \times (B^n_\xi)^\circ$, $\mathrm{WF}_{\mathrm{qsc}}$ propagates at finite speed under the flow of a vector field X given by rescaling geodesic flow; thus for $p \in \partial B^n_z \times (B^n_\xi)^\circ$ and T sufficiently small, $\mathcal{G}_T(p)$ is the point $\exp(-TX)[p] \in B^n_z \times (B^n_\xi)^\circ$. The vector field X blows up near the corner $\partial B^n_z \times \partial B^n_\xi$ in such a manner that certain integral curves reach in $\partial B^n_z \times \partial B^n_\xi$ in finite time at the "incoming normal points" $(\omega, -\omega)$ with $\omega \in \partial B^n = S^{n-1}$. Let $p \in B^n_z \times \partial B^n_\xi$ lie along a geodesic which as $t \to -\infty$ asymptotically has derivative $-\omega$. Then $\mathcal{G}_T(p) = \{\exp(-TX)[(\omega, -\omega)]\}$. Thus "singularities" (as measured by $\mathrm{WF}_{\mathrm{qsc}}$) originating in $\partial B^n_z \times (B^n_\xi)^\circ$ can leave $\partial B^n_z \times (B^n_\xi)^\circ$ through the corner and propagate across $(B^n_z)^\circ \times \partial B^n_\xi$ along geodesics, with infinite speed.

Just as the flow in $\partial B^n_z \times (B^n_\xi)^\circ$ can reach the incoming normal points in the corner at finite time, the "outgoing normal points" of the form (ω, ω) flow back into $\partial B^n_z \times (B^n_\xi)^\circ$. Suppose $\exp(sX)[(\omega, \omega)] = p$. Let $\mathsf{Scat}(\omega)$ denote all the points $\omega' \in \partial B^n$ such that there is a geodesic that asymptotically has derivative ω as $t \to +\infty$ and $-\omega'$ as $t \to -\infty$. For $T < s$, $\mathcal{G}_T(p) = \{\exp(-TX)[p]\}$, but for $T > s$,

$$\mathcal{G}_T(p) = \{\exp(-(T-s)X)[(\omega', -\omega')] : \omega' \in \mathsf{Scat}(\omega)\};$$

thus Scat describes the manner in which singularities scatter.

The structure of this paper is as follows. In §2 we discuss the geometric setting in which we shall work. In §3 we construct the scattering calculus of pseudodifferential operators, following Melrose [15]. In §4, we use the scattering calculus to define the quadratic-scattering calculus, and in §6–§9 we discuss the properties of these two calculi. In §10 we discuss background material on the Schrödinger equation and sketch the positive commutator arguments to be employed later. In §11 we discuss the "bicharacteristic flow" along which the qsc wavefront set propagates. In §12 we state the main theorems of the paper. We prove these theorems by constructing symbols of qsc pseudodifferential operators with specified convexity properties with respect to bicharacteristic flow (§13) and then employing a positive-commutator argument (§14).

I am very grateful to Richard Melrose for his generous advice and encouragement. I am also grateful to Walter Craig, Thomas Kappeler, and Walter Strauss for helpful discussions and for the preprint of [4]. Andras Vasy taught me much about the scattering calculus, and provided useful comments on the manuscript. The comments of an anonymous referee were also extremely helpful. This work was supported by a fellowship from the Fanny and John Hertz Foundation.

2. Geometric preliminaries

Let M be a compact manifold with boundary. We say that a function x is a *boundary defining function* for M if x is a positive smooth function on M such that $x = 0$ exactly on ∂M and $dx \neq 0$ on ∂M. Following Melrose [15], we define a *scattering metric* to be a Riemannian metric g on M such that for some choice of boundary defining function x, we have

$$g = \frac{dx^2}{x^4} + \frac{h}{x^2}$$

in a neighborhood of ∂M, where $h \in \mathcal{C}^\infty(\mathrm{Sym}^2(T^*M))$ is nondegenerate on ∂M (i.e. $h|_{\partial M}$ is a metric).

The main motivation for considering scattering metric is that this class of metrics includes asymptotically Euclidian ones: let RC denote the "radial compactification" map[1] from $\mathbb{R}^n_z$ to $\mathbb{R}^{n+1}$ with coordinates $(t_0, \dots, t_n) = (t_0, t')$, given by

$$\mathrm{RC} : z \mapsto \left(\frac{1}{\langle z \rangle}, \frac{z}{\langle z \rangle} \right).$$

where $\langle z \rangle = (1 + |z|^2)^{\frac{1}{2}}$. The image of $\mathbb{R}^n$ under this map is the interior of S^n_+, the upper hemisphere of the unit n-sphere in $\mathbb{R}^{n+1}$. Note that the manifold S^n_+ is diffeomorphic to the n-ball B^n. The function

$$x = (\mathrm{RC}^{-1})^*(|z|^{-1}) = \frac{t_0}{(1 - t_0^2)^{\frac{1}{2}}}$$

is a boundary defining function for S^n_+; it is a well-defined function near ∂S^n_+ which we can extend smoothly across $z=0$. We identify a neighborhood of ∂S^n_+ with $[0, \infty) \times S^{n-1}$ by mapping

$$t \mapsto \left(\frac{t_0}{(1 - t_0^2)^{\frac{1}{2}}}, \frac{t'}{(1 - t_0^2)^{\frac{1}{2}}} \right) = (x, \omega).$$

Under this identification,

$$(\mathrm{RC}^{-1})^*(dz^2) = \frac{dx^2}{x^4} + \frac{d\omega^2}{x^2}$$

[1] In [15], Melrose refers to this map as "stereographic compactification" and writes it "SP."

where $d\omega^2$ is the standard "round" metric on S^{n-1}. Thus if we replace $\mathbb{R}^n$ by its compactification, the Euclidian metric becomes a scattering metric; the class of scattering metrics on S^n_+ includes many metrics that are asymptotically Euclidian, as well as others that asymptotically look like *non-round* metrics on S^{n-1}.

For the duration of this paper, M is an n-dimensional manifold with boundary with boundary defining function x, endowed with a scattering metric g and a product-structure near the boundary, i.e. a diffeomorphism of $\overline{(\mathbb{R}_x)_+} \times \partial M$ with a neighborhood of ∂M. We will let y denote either a point in ∂M or the image of such a point in local coordinates on ∂M, depending on the context. Thus, using the product structure, $x, y_1, \dots, y_{n-1}$ furnish local coordinates on M near ∂M.

3. The scattering calculus

The calculus of pseudodifferential operators best suited to the Schrödinger equation is most easily defined in terms of the scattering calculus. On $\mathbb{R}^n$, the scattering calculus is the same as that used by Craig, Kappeler, and Strauss in [4]. It has a fairly long history, having been studied on $\mathbb{R}^n$ by Shubin [24], Parenti [19], and Cordes [2]; it is also the Weyl calculus for the metric

$$\frac{|dz|^2}{1+|z|^2} + \frac{|d\xi|^2}{1+|\xi|^2}$$

(see [10]). On manifolds it has been discussed by Schrohe [20], [21], Melrose [15], and Melrose and Zworski [18]. We will describe the iterated blowup approach to this calculus espoused in [15], which has the advantage of manifest coordinate invariance, and makes the later transition to the quadratic scattering calculus reasonably natural.

The Schwartz kernels of scattering pseudodifferential operators on $\mathbb{R}^n$ are of the form

$$\frac{1}{(2\pi)^n} \int e^{i(z-z')\cdot\xi} a(z,\xi)\, d\xi \tag{3.1}$$

where a satisfies the symbol estimates

$$\left| D_z^\alpha D_\xi^\beta a(z,\xi) \right| \leqslant C_{\alpha,\beta} \langle z \rangle^{-l-|\alpha|} \langle \xi \rangle^{m-|\beta|}. \tag{3.2}$$

Let $\dot{\mathcal{C}}^\infty(M)$ denote smooth functions on M vanishing to infinite order at ∂M. Then $\mathrm{RC}^*(\dot{\mathcal{C}}^\infty(S^n_+)) = \mathcal{S}(\mathbb{R}^n)$, and $(\mathrm{RC}^{-1})^*$ is well-defined on $\mathcal{S}(\mathbb{R}^n)$ and inverts RC^*.

Definition 3.1. The calculus of "scattering conormal operators" of multiorder (m, l) on S^n_+, denoted $\Psi^{m,l}_{\mathrm{scc}}(S^n_+)$, consists of operators $\dot{\mathcal{C}}^\infty(S^n_+) \to \dot{\mathcal{C}}^\infty(S^n_+)$ of the form

$$\phi \mapsto (\mathrm{RC}^{-1})^* \circ A \circ \mathrm{RC}^*(\phi)$$

where A has Schwartz kernel given by (3.1) with symbol satisfying (3.2).

Remark. The "scc" subscript stands for "scattering conormal," as distinct from "classical" or polyhomogeneous. Since the distinction is immaterial for the purposes of this paper, we shall not bother with distinguishing the classical subalgebra.

The scattering calculus is designed to be a microlocalization of certain vector fields.

Definition 3.2. The Lie algebra of $\mathfrak{b}$-*vector fields*, denoted $\mathcal{V}_b(M)$, is the space of vector fields tangent to ∂M. The Lie algebra of *scattering vector fields* is

$$\mathcal{V}_{sc}(M) = x\mathcal{V}_b(M).$$

The *scattering differential operators* are the differential operators given by smooth linear combinations of products of scattering vector-fields. They are filtered by their order and denoted $\mathrm{Diff}^m_{sc}(M)$. The $\mathfrak{b}$-differential operators $\mathrm{Diff}^m_b(M)$ are defined analogously. If V is a smooth vector bundle, we can also define b- and scattering differential operators acting on sections of V, denoted $\mathrm{Diff}^m_b(M;V)$ and $\mathrm{Diff}^m_{sc}(M;V)$ respectively.

Remarks. 1. The space $\mathcal{V}_b(M)$ is locally spanned over $\mathcal{C}^\infty(M)$ by $x\partial_x$ and ∂_y; $\mathcal{V}_{sc}(M)$ is spanned by $x^2\partial_x$ and $x\partial_y$.

2. One reason for considering scattering vector-fields is that $(\mathrm{RC}^{-1})^*$ takes *constant* vector fields on $\mathbb{R}^n$ into $\mathcal{V}_{sc}(S^n_+)$. The scattering vector fields are exactly those smooth vector fields which have finite norm in a scattering metric, and the Laplace-Beltrami operator for a scattering metric on M lies in $\mathrm{Diff}^2_{sc}(M)$.

There is an invariant definition of the scattering calculus in terms of iterated blowups that works on any manifold with boundary M. First, we need to define conormal distributions on manifolds with corners:

Definition 3.3. Let X be a compact manifold with corners and Y a p-submanifold (this means that in local coordinates, X and Y have a common decomposition as products of half-lines and lines; see [15] or [17]) with $\operatorname{codim} Y = s$. Let $\mathfrak{a}$ be a multi-index, assigning a real number to each boundary hypersurface of X. Let x_i be a defining function for the i'th boundary face, with $x^\mathfrak{a}$ denoting the appropriate product of powers of defining functions. Let V be a vector bundle over X.

Let $\dot{\mathcal{C}}^\infty(X;V)$ denote smooth sections of V vanishing to infinite order at all boundary hypersurfaces $x_i = 0$. Let $\mathcal{C}^{-\infty}(X;V) = [\dot{\mathcal{C}}^\infty(X;V^* \otimes \Omega X)]'$, where ΩX is the density bundle of X.

The space of distributions on X with values in V, conormal to the boundary of X with index $\mathfrak{a}$ is

$$\mathcal{A}^\mathfrak{a}(X;V) = \{u \in \mathcal{C}^{-\infty}(X;V) : \mathrm{Diff}^k_b(X;V)u \in x^\mathfrak{a}L^\infty(X) \text{ for all } k \in \mathbb{Z}^+\}.$$

The space of distributions on X with values in V, conormal with respect to the boundary with index $\mathfrak{a}$ and conormal with respect to Y of order m is denoted $\mathcal{A}^\mathfrak{a}I^m(X,Y;V)$ and consists of all distributions $u \in \mathcal{C}^{-\infty}(X;V)$ such that

1. Away from Y,

$$\mathrm{Diff}^k_b(X;V)u \in x^\mathfrak{a}L^\infty_{loc} \quad \text{for all } k \in \mathbb{Z}^+,$$

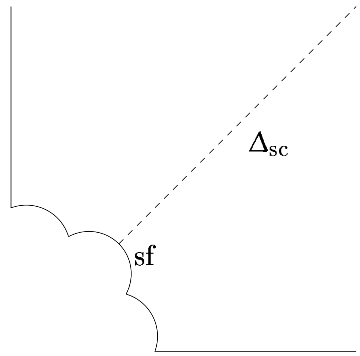

FIGURE 1. The scattering double-space M^2_{sc}, for a one-dimensional manifold M with boundary.

2. in the interior of X, u is conormal to Y of order m in the sense of Hörmander [9], and
3. near $Y \cap \partial X$, in coordinates (x, y', y'') for X such that $Y = \{y' = 0\}$ and in a local trivialization of V, we can write

$$u = \int e^{iy'\cdot\xi'} a(x, y'', \xi') d\xi'$$

where a satisfies the symbol estimates

$$\left|(xD_x)^\alpha (D_{y''})^\gamma (D_{\xi'})^\beta a(x, y'', \xi')\right| \leqslant C_{\alpha,\beta,\gamma} x^a \langle\xi\rangle^{m-s/2+n/4-|\beta|}.$$

Let $[X; Y]$ denote the smooth manifold with corners X blown up along the p-submanifold Y. We set $M^2_b = [M^2; (\partial M)^2]$. Let Δ_b denote the lift to M^2_b of the diagonal in M^2—in other words, Δ_b is the closure in M^2_b of the preimage under the blow-down map of the interior part of the diagonal. Now set $M^2_{sc} = [M^2_b; \partial\Delta_b]$; let Δ_{sc} be the lift of the diagonal to M^2_{sc}, and let sf denote the front face of the blowup and x_{sf} a defining function for it. We define the "scattering half-density bundle" ${}^{sc}\Omega(M) = x^{-1-n}\Omega M$, where ΩM is the usual density bundle. We define the "kernel density bundle"

$${}^{sc}KD^{\frac{1}{2}} = x_{sf}^{-\frac{1}{2}(n+1)} \Omega^{\frac{1}{2}}(M^2_{sc}).$$

Definition 3.4 (Invariant definition of scattering calculus)**.** The calculus of scattering conormal operators (acting on scattering half-densities) is defined by the Schwartz kernels of its elements, lifted from M^2 to M^2_{sc}:

$$\Psi^{m,l}_{scc}(M; {}^{sc}\Omega^{\frac{1}{2}}) = \left\{A \in \mathcal{A}^l I^m(M^2_{sc}, \Delta_{sc}; {}^{sc}KD^{\frac{1}{2}}) : A \equiv 0 \text{ at } \partial M^2_{sc} \backslash \mathrm{sf}\right\}$$

where l is the conormal index at the front face sf of the blowup $[M^2_b; (\partial M)^2]$.

More generally, for any vector bundles E and F over M, we define

$$\Psi^{m,l}_{scc}(M;E,F) = \Big\{A \in \mathcal{A}^l I^m \Big(M^2_{sc}, \Delta_{sc}; {}^{sc}KD^{\frac{1}{2}} \otimes \beta^* \operatorname{Hom}\Big[\pi_L^*(E \otimes {}^{sc}\Omega^{-\frac{1}{2}}), \pi_R^*(F \otimes {}^{sc}\Omega^{-\frac{1}{2}})\Big]\Big) : A \equiv 0 \text{ at } \partial M^2_{sc} \backslash \mathrm{sf}\Big\}.$$

where π_L and π_R are projections of M^2 on left and right factors, and $\beta : M^2_{sc} \to M^2$ is the total blow-down map. We write $\Psi^{m,l}_{scc}(M;E)$ for $\Psi^{m,l}_{scc}(M;E,E)$ and $\Psi^{m,l}_{scc}(M)$ for $\Psi^{m,l}_{scc}(M;\mathbb{C})$.

It is proven in §22 of [15] that on S^n_+, this definition agrees with Definition 3.1.

The scattering pseudodifferential operators are a microlocalization of the $\mathcal{V}_{sc}(M)$:

Proposition 3.5. *For all* $m, l \in \mathbb{R}$,

$$x^l \mathrm{Diff}^m_{sc}(M) \subset \Psi^{m,l}_{scc}(M).$$

The residual space $\Psi^{-\infty,\infty}_{scc}(M)$ consists of operators whose kernels are in $\dot{\mathcal{C}}^\infty(M \times M; \pi_R^*\Omega)$.

4. The quadratic-scattering calculus

Craig, Kappeler, and Strauss [4] have fruitfully investigated microlocal smoothness of solutions of the Schrödinger equation using the scattering algebra (see the remarks in §12 for a brief discussion of the results of [4]). We will instead use a related algebra of pseudodifferential operators that is more suited to proving time-dependent results.

Let M_q be the manifold obtained by changing the boundary-defining function on M to $\rho = x^2$, and hence changing the $\mathcal{C}^\infty$ structure on M (q is for "quadratic"). The interiors of M and M_q are canonically diffeomorphic, but the canonical diffeomorphism does not extend smoothly to the boundary. Instead, we merely have a smooth map

$$\Theta : M \to M_q$$

which is 1-1 and onto but which fails to have a smooth inverse. Note, though, that $\Theta^* : \mathcal{C}^{-\infty}(M_q) \to \mathcal{C}^{-\infty}(M)$ is an isomorphism.

The $\mathcal{C}^\infty$ structure on M_q *does* depend on the choice of boundary definining function x and the product structure near ∂M. For example, if we take some other choice of defining function $\bar{x}$, then $\bar{\rho} = \bar{x}^2$ will be a smooth function of $(\sqrt{\rho}, y)$, but *not* in general of (ρ, y), hence M_q with defining function ρ and $\overline{M}_q$ with defining function $\bar{\rho}$ are not canonically diffeomorphic.

Non-uniqueness of the choice of M_q notwithstanding, we select some M_q and define

$$\Psi^{m,l}_{qsc}(M;E,F) = \Theta^* \circ \Big[\Psi^{m,(l-m)/2}_{scc}(M_q; (\Theta^{-1})^*E, (\Theta^{-1})^*F)\Big] \circ (\Theta^*)^{-1}.$$

Remarks.

1. By the homotopy property of vector bundles, the bundles E and F can be arranged to have transition functions that are independent of x in some collar neighborhood of ∂M; thus, $(\Theta^{-1})^*E$ and $(\Theta^{-1})^*F$ are smooth vector bundles on M_q.
2. The reason for the apparently peculiar indexing of $\Psi^{m,l}_{\text{qsc}}(M)$ is that the filtration on $\Psi_{\text{scc}}(M)$ is psychologically convenient: if we radially compactify $\mathbb{R}^n$ to S^n_+, then constant coefficient differential operators on $\mathbb{R}^n$ are mapped to scattering vector fields. Also, by definition, $|z|^l$ becomes x^{-l}. Thus we can think of an operator in $x^l(\mathcal{V}_{\text{sc}}(S^n_+))^m$ as a differential operator of order m with decay of order l. The filtration on $\Psi^{\cdot,\cdot}_{\text{scc}}(M)$ was chosen with this convention in mind.

   On the other hand, we have $\Theta_*^{-1}(\rho^2\partial_\rho) = \frac{1}{2}x^3\partial_x$ and $\Theta_*^{-1}\rho\partial_y = x^2\partial_y$. These vector fields are in $x\mathcal{V}_{\text{sc}}(M)$, and if we wish to maintain our sensible filtration, corresponding to orders of decay and differentiation on $\mathbb{R}^n$, we must assign to these vector fields the order $(1,1)$. Also, the operator of multiplication by ρ should manifestly have order $(0,2)$. Thus, we want to assign the order (m,l) to $\rho^{(l-m)/2}(\mathcal{V}_{\text{sc}}(M_q))^m$, and this fixes the indexing given above for Ψ_{qsc}.
3. As a result of our choice of indexing, for any $l \in \mathbb{R}$,
$$\bigcup_{m\in\mathbb{R}} \Psi^{m,l}_{\text{qsc}}(M) = \Psi^{\infty,-\infty}_{\text{qsc}}(M)$$
   and
$$\bigcap_{m\in\mathbb{R}} \Psi^{m,l}_{\text{qsc}}(M) = \Psi^{-\infty,\infty}_{\text{qsc}}(M) = \Psi^{-\infty,\infty}_{\text{scc}}(M)$$
   We also have $\Psi^{m,l}_{\text{qsc}}(M) \subset \Psi^{m+1,l+1}_{\text{qsc}}(M)$ for all (m,l).

In the following section, we offer an invariant definition of Ψ_{qsc}, analogous to our general definition of Ψ_{sc}.

5. Invariant definition of the quadratic-scattering calculus

We recall from [17] or [6] that if X is a manifold with corners and Y a p-submanifold, and if S is a subbundle of N^*Y satisfying a cleanness condition, we can define the *parabolic blowup* of Y in X along S, denoted $[X,Y;S]$. In the simplest possible case, in which X is $\mathbb{R}^n$, Y is the origin, and S is a subspace of $(\mathbb{R}^n)^*$, we can define an $\mathbb{R}^+$ action M_δ on $\mathbb{R}^n$ as follows: let $S^0 \subset \mathbb{R}^n$ be the annihilator of S, and let T be a complement of S^0 in $\mathbb{R}^n$. Thus every $v \in \mathbb{R}^n$ can be uniquely written $v = s + t$. We set $M_\delta(v) = (\delta^2 s + \delta t)$. Now let ff (for "front face") be the non-round sphere $(\mathbb{R}^n\backslash 0)/\mathbb{R}_+$. We define the S-parabolic blowup of 0 in $\mathbb{R}^n$ to be ff $\sqcup\, \mathbb{R}^n\backslash 0$. In [6], this definition is shown to be independent of the choice of T, and is extended successively to cover the blowup of the zero section of a vector-bundle, of a submanifold of a manifold with boundary, and of a submanifold of a manifold with corners.

We can now define a "qsc double-space" analogous to M^2_{sc} as follows: set $M^2_b = [M^2;(\partial M)^2]$ and let Δ_b denote the lift to M^2_b of the diagonal in M^2. Let $S = N^*_{\partial\Delta_b}\Delta_b$.

We proceed as in the scattering case, but blow up parabolically instead of spherically: $M^2_{\mathrm{qsc}} = [M^2_b; \partial\Delta_b, S]$. We define the "qsc density bundle" ${}^{\mathrm{qsc}}\Omega(M) = x^{-1-2n}\Omega M$ and the "qsc kernel density bundle"

$$ {}^{\mathrm{qsc}}\mathrm{KD}^{\frac{1}{2}} = x_{\mathrm{qsf}}^{-\frac{1}{2}(2n+1)}\Omega^{\frac{1}{2}}(M^2_{\mathrm{qsc}}). $$

where qsf denotes the front face of the blowup $[M^2_b; \partial\Delta_b, S]$ and x_{qsf} is the defining function for this boundary face. Let Δ_{qsc} be the lift of the diagonal to M^2_{qsc}. Let $\tilde{\Theta}$ denote the lift of the canonical map $\Theta : (M^2)^\circ \to (M^2_q)^\circ$ to a map $(M^2_{\mathrm{qsc}})^\circ \to ((M_q)^2_{\mathrm{sc}})^\circ$

Proposition 5.1. *The following maps are isomorphisms:*

1.
$$ \Theta^* : {}^{\mathrm{sc}}\Omega^{\frac{1}{2}}(M_q) \to {}^{\mathrm{qsc}}\Omega^{\frac{1}{2}}(M) $$

2.
$$ (\tilde{\Theta})^* : {}^{\mathrm{sc}}\mathrm{KD}^{\frac{1}{2}}((M_q)^2_{\mathrm{sc}})\Big|_{(\mathrm{sf})^\circ} \to {}^{\mathrm{qsc}}\mathrm{KD}^{\frac{1}{2}}(M^2_{\mathrm{qsc}})\Big|_{(\mathrm{qsf})^\circ} $$

3.
$$ (\tilde{\Theta})^* : \Psi^{m,l}_{\mathrm{scc}}(M_q; {}^{\mathrm{sc}}\Omega^{\frac{1}{2}}) \to \left\{ A \in \mathcal{A}^{2l} I^m(M^2_{\mathrm{qsc}}, \Delta_{\mathrm{qsc}}; {}^{\mathrm{qsc}}\mathrm{KD}^{\frac{1}{2}}) : A \equiv 0 \textit{ at } \partial M^2_{\mathrm{qsc}} \backslash \mathrm{qsf} \right\}. $$

Thus we could have directly defined

$$ \Psi^{m,l}_{\mathrm{qsc}}(M; {}^{\mathrm{qsc}}\Omega^{\frac{1}{2}}) = \left\{ A \in \mathcal{A}^{l-m} I^m(M^2_{\mathrm{qsc}}, \Delta_{\mathrm{qsc}}; {}^{\mathrm{qsc}}\mathrm{KD}^{\frac{1}{2}}) : A \equiv 0 \text{ at } \partial M^2_{\mathrm{qsc}} \backslash \mathrm{qsf} \right\}, \tag{5.1} $$

and extended this definition to arbitrary vector bundles as above.

Proof. 1. We have $\Theta^* : {}^{\mathrm{sc}}T^*M_q \to {}^{\mathrm{qsc}}T^*M$, and ${}^{\mathrm{sc}}\Omega = |\wedge^n|({}^{\mathrm{sc}}T^*)$, ${}^{\mathrm{qsc}}\Omega = |\wedge^n|({}^{\mathrm{qsc}}T^*)$.

2. First we write out coordinates near the front faces of the two double-spaces: Let (x, y) and (x', y') be the coordinates for the two factors of M in M^2. Let $\rho = x^2$ and $\rho' = (x')^2$. If $s = x/x'$ then we can take x', s, y, y' as coordinates near Δ_b on the front face of M^2_b. We can use $\rho', \bar{s}, y, y'$ as coordinates on the front face of $(M_q)^2_b$, where $\bar{s} = \rho/\rho' = s^2$. Δ_b is defined by $s = 1$, $y = y'$ in M^2_b, so on the front face qsf of M^2_{qsc} we introduce coordinates $X = (s-1)/(x')^2$ and $Y = (y - y')/(x')^2$; the coordinate system for M^2_{qsc} is now (x', X, y', Y), with x' defining the front face qsf. On $(M_q)^2_b$, Δ_b is defined by $\bar{s} = 1$, $y = y'$, so on the front face sf of $(M_q)^2_{\mathrm{sc}}$ we set $\bar{X} = (\bar{s} - 1)/\rho'$ and $\bar{Y} = (y - y')/\rho'$; the coordinates for $(M_q)^2_{\mathrm{sc}}$ are now $(\rho', \bar{X}, y', \bar{Y})$, with ρ' defining sf. Thus $(\tilde{\Theta})^*\bar{X} = X(1+s)$ and $(\tilde{\Theta})^*\bar{Y} = Y$ (note that $1 + s$ is a smooth, nonvanishing function).

In the coordinates we have introduced, $(\rho')^{-\frac{1}{2}(n+1)}\left|d\rho' d\bar{X} dy' d\bar{Y}\right|^{\frac{1}{2}}$ is a smooth, nonvanishing section of ${}^{\mathrm{qsc}}\mathrm{KD}^{\frac{1}{2}}(M_q)^2_{\mathrm{sc}}$, and the above remarks show that it pulls back to a nonvanishing multiple of $(x')^{-n-\frac{1}{2}}|dx' dX dy' dY|^{\frac{1}{2}}$.

3. By definition, an element $A \in \Psi^{m,l}_{scc}(M_q; {}^{sc}\Omega^{\frac{1}{2}})$ can be written, in a neighborhood of $\Delta_{sc} \cap \mathrm{sf}$ and using the coordinates introduced above, as

$$A = \frac{\omega}{(2\pi)^n} \int e^{i(\bar{X}\xi_1 + \bar{Y}\cdot\xi')} a(\rho', y', \xi) d\xi,$$

where $\xi' = (\xi_2, \dots, \xi_n)$, ω is a smooth section of ${}^{sc}KD^{\frac{1}{2}}$, and a satisfies the symbol estimates

$$\left|(\rho' D_{\rho'})^{\alpha} (D_{y'})^{\beta} (D_{\xi})^{\gamma} a\right| \leqslant C_{\alpha,\beta,\gamma} (\rho')^{l} \langle \xi \rangle^{m-|\beta|} \tag{5.2}$$

(here we are identifying the operator A and its Schwartz kernel). Thus,

$$(\tilde{\Theta})^* A = \frac{(\tilde{\Theta})^* \omega}{(2\pi)^n} \int e^{i((1+s)X\xi_1 + Y\cdot\xi')} a((x')^2, y', \xi) d\xi. \tag{5.3}$$

Since $(1+s)$ is nonvanishing at $X = 0$, by classical results of Hörmander [9], (5.3) is the representation of an arbitrary conormal distribution with respect to Δ_{qsc}. The new symbol $a((x')^2, y', \xi)$ satisfies (5.2) with ρ' replaced by x' and with order $2l$ instead of l. □

Remark. It is straightforward to compute, e.g. in the coordinates used above for M^2_{qsc} and analogous ones for M^2_{sc}, that in fact

$$\Psi^{m,l}_{qsc}(M; {}^{qsc}\Omega^{\frac{1}{2}}) \subset \Psi^{m,l}_{sc}(M; {}^{sc}\Omega^{\frac{1}{2}}).$$

This inclusion is not particularly useful, however.

For the study of Schrödinger operators, we will want a "parameter-dependent" version of $\Psi_{qsc}(M)$, but we only require the crudest notion of parameter dependence.

Definition 5.2. A one-parameter family of operators $A(t)$ is said to be in the algebra

$$\Psi^{m,l}_{qsc}(M; {}^{qsc}\Omega^{\frac{1}{2}})$$

if the Schwartz kernels of $A(t)$ lie in

$$\mathcal{C}^\infty(\mathbb{R}_t; \mathcal{A}^{l-m} I^m(M^2_{qsc}, \Delta_{qsc}; {}^{qsc}KD^{\frac{1}{2}})),$$

where the topology on $\mathcal{A}^{l-m} I^m(M^2_{qsc}, \Delta_{qsc}; {}^{qsc}KD^{\frac{1}{2}})$ is the usual topology on conormal spaces, given by the best constants in the conormal estimates and symbol estimates of Definition 3.3.

(The definition can also be extended to arbitrary vector bundles in the usual manner.)

6. Symbol maps

The symbol map on $\Psi_{scc}^{m,l}(M)$ has two components. One component is essentially the same as the symbol map for pseudodifferential operators on a compact manifold. First we define it on $\mathcal{V}_{sc}(M)$. The vector fields $\mathcal{V}_{sc}(M)$ are actually sections of a smooth vector bundle ${}^{sc}TM$ over the manifold with boundary M. ${}^{sc}TM$ is spanned by $x^2\partial_x$ and $x\partial_y$ near ∂M; in the interior of M, it is canonically isomorphic to TM. The dual bundle to ${}^{sc}TM$, ${}^{sc}T^*M$, is spanned by the differentials dx/x^2 and dy/x near ∂M. Given $X \in \mathcal{V}_{sc}(M) = \mathcal{C}^\infty(M; {}^{sc}TM)$, we write $\sigma_{sc,1}(X) = iX$, where on the right-hand side, we consider X to be an element of $\mathcal{C}^\infty({}^{sc}T^*M)$, homogeneous of degree 1 in the fibers. We can extend this symbol map to a map

$$\sigma_{sc,m} : \mathrm{Diff}_{sc}^m(M) \to S^m({}^{sc}T^*M)/S^{m-1}({}^{sc}T^*M)$$

where $S^m({}^{sc}T^*M)$ denotes functions satisfying the usual Kohn-Nirenberg symbol estimates in the fibers; the range is actually contained in the homogeneous polynomials of order m. The map $\sigma_{sc,m}$ can be extended further to a principal symbol map on scattering pseudodifferential operators:

$$\sigma_{sc,m} : \Psi_{scc}^{m,l}(M) \to S^m({}^{sc}T^*M)/S^{m-1}({}^{sc}T^*M).$$

Example 6.1. Canonical dual coordinates α, β can be defined on ${}^{sc}T^*M$ by letting

$$\alpha dx/x^2 + \beta \cdot dy/x$$

denote the tautological one-form. Then $\sigma_{sc,1}(x^2\partial_x) = \alpha$ and $\sigma_{sc,1}(x\partial_y) = \beta$.

The symbol $\sigma_{sc,\cdot}$ gives useful information about an operator over the interior of M but does not provide sufficient information about its asymptotics near ∂M. For asymptotic information, we use the "normal homomorphism." Let $p \in \partial M$. Identifying the vector-space ${}^{sc}T_pM$ with first-order constant coefficient differential operators on itself, we obtain, for each $p \in \partial M$, a restriction map (obtained by "freezing coefficients")

$$N_{sc,p} : \mathcal{V}_{sc}(M) \to \mathrm{Diff}_I^1({}^{sc}T_pM)$$

where the I indicates translation-*invariant* differential operators in the fibers. Since

$$[\mathcal{V}_{sc}(M), \mathcal{V}_{sc}(M)] \subset x\mathcal{V}_{sc}(M),$$

we can extend $N_{sc,p}$ to a map

$$N_{sc,p} : \mathrm{Diff}_{sc}^m(M) \to \mathrm{Diff}_I^m({}^{sc}T_pM)$$

Invariant differential operators on a vector space are canonically identified with polynomials on its dual by the inverse Fourier transform. Thus we have a somewhat more convenient map

$$\widehat{N}_{sc} : \mathrm{Diff}_{sc}^m(M) \to S^m({}^{sc}T^*_{\partial M}M);$$

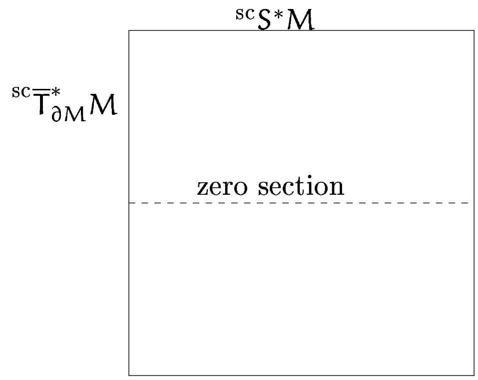

FIGURE 2. ${}^{sc}\overline{T}^*M$, for M a closed interval.

in fact the image is exactly the polynomials of order m in the fibers. We further extend to a map

$$\widehat{N}^l_{sc} : x^l \mathrm{Diff}^m_{sc}(M) \to x^l S^m({}^{sc}T^*_{\partial M}M).$$

The map $\widehat{N}^l_{sc}$ does have some relationship to $\sigma_{sc,m}$: if $P \in x^l \mathrm{Diff}^m_{sc}(M)$, then $\widehat{N}^l_{sc}(P) - \sigma_{sc,m}(P)$ is x^l times a polynomial of order $(m-1)$ in the fiber variables.

Example 6.2. In the coordinates used in Example 6.1, we have $\widehat{N}^l_{sc}(x^{l+2}\partial_x) = x^l\alpha$ and $\widehat{N}^l_{sc}(x^{l+1}\partial_y) = x^l\beta$.

The relationship between the symbols $\sigma_{sc,\cdot}$ and $\widehat{N}_{sc}$ is clearer if we compactify the bundle on which they live:

Definition 6.3. Let ${}^{sc}\overline{T}^*M$ be the compact manifold with corners obtained by radially compactifying the fibers of the bundle ${}^{sc}T^*M$. Let $C_{sc}(M) = \partial({}^{sc}\overline{T}^*M)$. Let ${}^{sc}S^*M$ denote the boundary face of ${}^{sc}\overline{T}^*M$ obtained by fiber compactification, and let ${}^{sc}\overline{T}^*_{\partial M}M$ denote the other boundary face, defined by $x = 0$.

The maps $\sigma_{sc,\cdot}$ and $\widehat{N}_{sc}$ must agree at the corner ${}^{sc}S^*M \cap {}^{sc}\overline{T}^*_{\partial M}M$.

Definition 6.4. Let

$$\mathcal{A}^{\{m,l\}}(C_{sc}M) = \mathcal{A}^{m,l}({}^{sc}\overline{T}^*M)/\mathcal{A}^{m-1,l+1}({}^{sc}\overline{T}^*M),$$

where m is the conormal index at the boundary face ${}^{sc}S^*M$ and l is the conormal index at ${}^{sc}\overline{T}^*_{\partial M}M$.

Remark. We employ the opposite sign convention on m from that used in §5 of [15].

Radial compactification of $\mathbb{R}^n$ takes symbols of order m to conormal distributions on S^n_+ with respect to ∂S^n_+ of order $-m$. Thus we can consider the combined symbol map, $j_{sc,m,l}$, defined on the operator $P \in x^l \mathrm{Diff}^m_{sc}(M)$ by

$$j_{sc,m,l}(P) = (\sigma_{sc,m}(P), \widehat{N}^l_{sc}(P))$$

as a map
$$x^l \mathrm{Diff}^m_{sc}(M) \to \mathcal{A}^{\{-m,l\}}(C_{sc}M).$$

The map $j_{sc,m,l}$ can be extended to all of $\Psi^{m,l}_{scc}$. (Note that for the non-classical algebra used here, we cannot simply define $j_{sc,m,l}(P) = (\sigma_{sc,m}(P), \widehat{N}^l_{sc}(P))$: in order to retain full information at the corner, we have to regard $j_{sc,\cdot}$ as defined by the Fourier transform of the Schwartz kernel in the normal bundle of Δ_{sc} modulo conormal distributions of higher order at both boundary faces of ${}^{sc}\overline{T}^*M$ simultaneously.) The following properties of the resulting joint symbol map are discussed in [15].

Proposition 6.5.

1. *There is a short exact sequence*
$$0 \to \Psi^{m-1,l+1}_{scc}(M) \to \Psi^{m,l}_{scc}(M) \xrightarrow{j_{sc,m,l}} \mathcal{A}^{\{-m,l\}}(C_{sc}M) \to 0.$$
2. *The symbol map is multiplicative.*
3. *The Poisson bracket extends continuously from the usual bracket defined on the interior of ${}^{sc}\overline{T}^*M$ to a Poisson bracket on $\mathcal{A}^{\{\cdot,\cdot\}}({}^{sc}\overline{T}^*M)$, and*
$$j_{sc,m_1+m_2-1,l_1+l_2+1}([P,Q]) = \frac{1}{i}\{j_{sc,m_1,l_1}(P), j_{sc,m_2,l_2}(Q)\}.$$

We wish to consider symbols of quadratic scattering ΨDO's. If $A \in \Psi^{m,l}_{qsc}(M)$ then
$$A = \Theta^* \circ P \circ (\Theta^*)^{-1}$$
for $P \in \Psi^{m,(l-m)/2}_{scc}(M_q)$. P has a joint symbol in $\mathcal{A}^{\{-m,(l-m)/2\}}(C_{sc}M_q)$. A natural approach is to pull back this symbol to M, and declare the result the qsc-symbol of P.

Definition 6.6. The quadratic scattering tangent bundle on M is the bundle ${}^{qsc}TM$ whose sections are vector fields in $x\mathcal{V}_{sc}(M)$. The qsc cotangent bundle, ${}^{qsc}T^*M$, is the dual of ${}^{qsc}TM$. The manifold with corners obtained by radially compactifying the fibers of ${}^{qsc}T^*M$ is denoted ${}^{qsc}\overline{T}^*M$, and $C_{qsc}M = \partial({}^{qsc}\overline{T}^*M)$. Let ${}^{qsc}S^*M$ denote the boundary face of ${}^{qsc}\overline{T}^*M$ obtained by fiber compactification, and let ${}^{qsc}\overline{T}^*_{\partial M}M$ denote the other boundary face, defined by $x = 0$.

Let
$$\mathcal{A}^{[m,l]}(C_{qsc}M) = \mathcal{A}^{m,l}({}^{qsc}\overline{T}^*M)/\mathcal{A}^{m-1,l+2}({}^{qsc}\overline{T}^*M).$$

Thus the bundle ${}^{qsc}T^*M$ is locally spanned by $\rho^2\partial_\rho = \frac{1}{2}x^3\partial_x$ and $\rho\partial_y = x^2\partial_y$.

The map $(\Theta^{-1})^*$ induces a pullback map from distributions on ${}^{sc}\overline{T}^*M_q$ to distributions on ${}^{qsc}\overline{T}^*M$. The pullback of $j_{sc,m,(l-m)/2}(P)$ under $(\Theta^{-1})^*$ is in $\mathcal{A}^{[-m,l]}(C_{qsc}M)$, hence this is the space of symbols for the qsc-calculus.

Proposition 6.7. *There is a joint symbol map*
$$j_{qsc,m,l} : \Psi^{m,l}_{qsc}(M) \to \mathcal{A}^{[-m,l-m]}(C_{qsc}M)$$
such that

1. *There is a short exact sequence*

$$0 \to \Psi_{qsc}^{m-1,l+1}(M) \to \Psi_{qsc}^{m,l}(M) \xrightarrow{j_{qsc,m,l}} \mathcal{A}^{[-m,l-m]}(C_{qsc}M) \to 0. \tag{6.1}$$

2. *The symbol map is multiplicative.*
3. *The Poisson bracket extends continuously from the usual bracket defined on the interior of* ${}^{qsc}\overline{T}^*M$ *to* $\mathcal{A}^{[\cdot,\cdot]}$*, and*

$$j_{qsc,m_1+m_2-1,l_1+l_2}([P,Q]) = \frac{1}{i}\{j_{qsc,m_1,l_1}(P), j_{qsc,m_2,l_2}(Q)\}.$$

This proposition follows from Proposition 6.5 by pullback.

Remark. The symbol $j_{qsc,\cdot}$ *is* well-defined, independent of choice of boundary defining function x; one could see this by proving the above theorem from scratch, in imitation of the construction of the symbol map on Ψ_{scc}.

Example 6.8. Let λ, μ be canonical coordinates in ${}^{qsc}T^*M$ such that the canonical one-form is $\lambda dx/x^3 + \mu \cdot dy/x^2$. Then we have

$$j_{qsc,1,0}(x^3 D_x) = \lambda$$

and

$$j_{qsc,1,0}(x^2 D_{y_i}) = \mu_i.$$

Example 6.9. Again, let λ, μ be canonical coordinates in ${}^{qsc}T^*M$ such that the canonical one-form is $\lambda dx/x^3 + \mu \cdot dy/x^2$. Recall that Δ denotes the Laplace-Beltrami operator with respect to the scattering metric g:

$$\Delta = \sum_{j,k=0}^{n} \frac{1}{\sqrt{g}} D_j g^{jk} \sqrt{g} D_k \tag{6.2}$$

in any coordinate system. If we take coordinates $z_0 = x$ and $z_j = y_j$ for $j = 1, \dots, n-1$, we have

$$\begin{aligned} g^{00} &= x^4 + O(x^6) \\ g^{0j} &= O(x^4) \\ g^{ij} &= x^2 \bar{h}^{ij} + O(x^3) \end{aligned} \tag{6.3}$$

where $\bar{h} = h|_{\partial M}$; thus, as observed in [15],

$$\begin{aligned} \Delta &\in (x^2 D_x)^2 + i(n-1)x^3 D_x + x^2 \Delta_0 + x^3 \mathrm{Diff}_b^2(M) \\ &= x^{-2}\left((x^3 D_x)^2 + inx^5 D_x + x^4 \Delta_0 + x^5 \mathrm{Diff}_b^2(M)\right) \end{aligned} \tag{6.4}$$

where Δ_0 is Laplace-Beltrami operator for $\bar{h}$, extended to M using the product structure at the boundary. Actually, we can say a bit more. The only D_x^2 term in Δ is $g^{00} D_x^2$. Thus the coefficient of D_x^2 in Δ is $x^4 + O(x^6)$.

Note that $x^5\mathrm{Diff}^2_b(M) \subset x\mathrm{Diff}^2_{qsc}(M)$ ($\mathrm{Diff}^m_{qsc}(M)$ consists of differential operators in $\Psi^{m,0}_{qsc}(M)$). Since the normal symbol is defined modulo *two* orders of vanishing, this term does contribute to the normal symbol. Since $x^5\mathcal{V}_b$ is annihilated under the normal symbol map, the normal symbol of the term $x^5\mathrm{Diff}^2_b(M)$ contributes only terms homogeneous in the fiber variables of order two, vanishing to first order in x. By the observations in the previous paragraph, the normal symbol of this error term is not just *any* homogeneous polynomial of order two, vanishing to first order in x, but in fact can be written $xr(\lambda, \mu)$, with

$$r(\lambda, \mu) \in x\mathcal{C}^\infty(x, y)\lambda^2 + \mathcal{C}^\infty(x, y)\lambda\mu + \mathcal{C}^\infty(x, y)\mu^2 \tag{6.5}$$

where the indices have been left off of μ for brevity.

We have now shown that

$$\widehat{N}^0_{qsc}(\Delta) = \frac{1}{x^2}\left(\lambda^2 + |\mu|^2 + xr(\lambda, \mu)\right)$$

where $|\mu|^2$ is the norm of $\mu \cdot dy$ with respect to the metric $\bar{h}$, and $r(\lambda, \mu)$ is of the form (6.5).

By the same token, we may throw out terms in (6.4) of degree lower than two and conclude that

$$\sigma_{qsc,2}(\Delta) = \frac{1}{x^2}\left(\lambda^2 + |\mu|^2 + xr(\lambda, \mu)\right).$$

Note that the interior and normal symbols of a differential operator generally do not agree as polynomials—the Laplacian is atypical in this respect; see the remarks following the proof of Lemma 3 in [15].

The joint symbol of Δ is thus represented in $\mathcal{A}^{[-2,-2]}(C_{qsc}M)$ by

$$j_{qsc,2,0}(\Delta) = \frac{1}{x^2}\left(\lambda^2 + |\mu|^2 + xr(\lambda, \mu)\right); \quad r \text{ satisfies } (6.5). \tag{6.6}$$

For the remainder of this section, $*$ stands for sc(c) or qsc.

Definition 6.10. An operator $P \in \Psi^{m,l}_*(M)$ is said to be *elliptic* at a point $p \in C_*M$ if $j_{*,m,l}(p)$ is nonzero. The set of points at which P is elliptic is denoted $\mathrm{ell}_{*,m,l} P$. If P is elliptic everywhere, it is simply said to be *elliptic.*

(Following convention, we shall omit the subscripts on ell; the algebra and order will always be clear from context.)

Definition 6.11. Let P be an element of $\Psi^{m,l}_*(M)$. A point $p \in C_*M$ is in the complement of WF'_*P (the *operator wavefront set* of P) if there exists $Q \in \Psi^{-m,-l}_*(M)$ such that Q is elliptic at p and $PQ \in \Psi^{-\infty,\infty}_*(M)$.

Proposition 6.12. *For* $A, B \in \Psi_*(M)$, $\mathrm{WF}'_*AB \subset \mathrm{WF}'_*A \cap \mathrm{WF}'_*B$ *and* $\mathrm{WF}'_*A^* = \mathrm{WF}'_*A$.

Proposition 6.13. *If* $P \in \Psi_*^{m,l}(M)$ *is elliptic at* $p \in C_*M$ *then there exists* $Q \in \Psi_*^{-m,-l}(M)$ *such that*

$$p \notin \mathrm{WF}_*'(PQ - I).$$

This proposition can be proved in the same way as Theorem 18.1.24' of [10].

The following proposition is a variant of Proposition 6.13 that we will use in our positive commutator estimates.

Proposition 6.14. *If* $C \in \Psi_*^{m,l}(M)$ *is and* $E \in \Psi_*^{2m,2l}(M)$ *with* $\mathrm{WF}_*'E \subset \mathrm{ell}\, C$*, then there exists* $Q \in \Psi_*^{0,0}(M)$ *such that*

$$E - C^*QC \in \psi_*^{-\infty,\infty}(M).$$

For the proof, see the analogous Lemma 5.5 of [4].

7. Quantization

We can construct a continuous, linear map

$$\mathrm{Op} : \mathcal{A}^{-\infty,-\infty}({}^{qsc}\overline{T}^*M) \to \Psi_{qsc}^{\infty,-\infty}(M)$$

with

$$\mathrm{Op} : \mathcal{A}^{-m,l-m}({}^{qsc}\overline{T}^*M) \to \Psi_{qsc}^{m,l}(M)$$

as follows. Let ω be the symplectic form on ${}^{qsc}T^*M$. Given $a \in \mathcal{A}^{-m,l-m}({}^{qsc}\overline{T}^*M)$, let $\breve{a}$ denote the inverse Fourier transform of $a\omega^n$ in the fiber variables; thus,

$$\breve{a} \in \mathcal{A}^{l-m}I^m({}^{qsc}\overline{T}M, 0; \pi^*({}^{qsc}\Omega))$$

where π denotes the projection map for the bundle ${}^{qsc}\overline{T}^*M$ and 0 denotes the zero section.

Let $\pi^2_{qsc,L}$ and $\pi^2_{qsc,R}$ denote the maps $M^2_{qsc} \to M$ given by blowdown to M^2 followed by projection onto the left or right factor. A computation in the coordinates used in the proof of Proposition 5.1 shows that $(\pi^2_{qsc,L})_*$ is an isomorphism between $N\Delta_{qsc}$ and ${}^{qsc}TM$, and induces a natural diffeomorphism between qsf and ${}^{qsc}\overline{T}_{\partial M}M$; by symmetry, the same is true for $(\pi^2_{qsc,R})_*$. By the Tubular Neighborhood Theorem, $N\Delta_{qsc}$ is diffeomorphic to a neighborhood of Δ_{qsc} in M^2_{qsc}, with the zero-section mapping to Δ_{qsc} and $(N\Delta_{qsc})|_{qsf}$ to $(\mathrm{qsf})^\circ$. We can combine this diffeomorphism with the bundle equivalence above to obtain a diffeomorphism j between an open neighborhood U of $\Delta_{qsc} \cup \mathrm{qsf}$ with an open neighborhood V of the zero section and ${}^{qsc}\overline{T}_{\partial M}M$ in ${}^{qsc}\overline{T}M$ such that $\pi \circ j = \pi^2_{qsc,R}$ on Δ_{qsc}. Now let ϕ be a smooth function on ${}^{qsc}\overline{T}M$ equal to zero outside V and one on a smaller neighborhood of the zero section and ${}^{qsc}T^*_{\partial M}M$. Then we can set

$$\mathrm{Op}(a) = j^*(\phi\breve{a}) \in \mathcal{A}^{l-m}I^m(M^2_{qsc}, \Delta_{qsc}; (\pi^2_{qsc,R})^*({}^{qsc}\Omega)) = \Psi^{m,l}_{qsc}(M).$$

Proposition 7.1. *The quantization* Op *is a continuous linear map* $\mathcal{A}^{-\infty,-\infty}({}^{qsc}\overline{T}^*M) \to \Psi_{qsc}^{\infty,-\infty}(M)$ *enjoying the following properties*

1. $j_{qsc,m,l} \circ \mathrm{Op} : \mathcal{A}^{-m,l-m}(M) \to \mathcal{A}^{[-m,l-m]}(M)$ *is the natural projection map.*

2. *If* a_n *is a bounded sequence in* $\mathcal{A}^{0,0}(M)$ *and* $a_n \to a$ *in some* $\mathcal{A}^{p,q}(M)$*, then* $\mathrm{Op}(a_n) \to \mathrm{Op}(a)$ *in the strong operator topology on* $\mathcal{B}(L^2(M))$.
3. $\mathrm{WF}'_{\mathrm{qsc}} \mathrm{Op}(a) = \mathrm{ess\,supp}\, a$*, where* $\mathrm{ess\,supp}(a)$*, the essential support of* a*, is the set of points in* $C_{\mathrm{qsc}}M$ *near which* a *is not in* $\dot{\mathcal{C}}^\infty({}^{\mathrm{qsc}}\overline{T}^*M)$.

An analogous construction yields the same result for the scattering calculus (cf. [15]).

8. Sobolev spaces

Let $L^2(M)$ denote functions on M that are square-integrable with respect to the volume element defined by the scattering metric g. Let $*$ stand for sc(c) or qsc.

The basic boundedness result is the following:

Proposition 8.1. $\Psi_*^{0,0}(M)$ *is bounded on* $L^2(M)$.

This proposition follows from the proof of Hörmander's boundedness theorem in [9].

Definition 8.2. The scattering and quadratic-scattering Sobolev spaces are defined by

$$H_*^{m,l}(M) = \left\{ u \in \mathcal{C}^{-\infty}(M) : \Psi_*^{m,-l}(M)u \in L^2(M) \right\}.$$

Note the minus sign in the indexing chosen for the Sobolev spaces. As a result, increasing indices mean increasing decay and regularity, so $H_{\mathrm{sc}}^{m,l}(M) \subseteq H_{\mathrm{sc}}^{m',l'}(M)$ and $H_{\mathrm{qsc}}^{m,l}(M) \subseteq H_{\mathrm{qsc}}^{m',l'}(M)$ for $m' \leqslant m$ and $l' \leqslant l$,

$$H_{\mathrm{qsc}}^{\infty,\infty}(M) = H_{\mathrm{sc}}^{\infty,\infty}(M) = \dot{\mathcal{C}}^\infty(M), \tag{8.1}$$

and

$$H_{\mathrm{qsc}}^{-\infty,-\infty}(M) = H_{\mathrm{sc}}^{-\infty,-\infty}(M) = \mathcal{C}^{-\infty}(M). \tag{8.2}$$

A version of Proposition 8.1 is, of course, true a bit more generally:

Proposition 8.3. *Let* $A \in \Psi_*^{m',l'}(M)$*. Then*

$$A : H_*^{m,l}(M) \to H_*^{m-m',l+l'}(M)$$

is continuous for any m, l.

Lemma 8.4. *Let* $A \in \Psi_*^{2m,-2l}(M)$ *be elliptic, self-adjoint, and strictly positive. Then* $\langle A\cdot,\cdot\rangle^{\frac{1}{2}}$ *is equivalent to the norm on* $H_*^{m,l}(M)$.

The proof follows easily from Proposition 2.2.2 of [9].

An interpolation lemma for sc Sobolev spaces will be useful.

Lemma 8.5. *For all* (m_1, l_1), (m_2, l_2)*, and*

$$(m, l) = (sm_1 + (1-s)m_2, sl_1 + (1-s)l_2)$$

with $s \in [0,1]$*, there is a continuous embedding*

$$H_{\mathrm{sc}}^{m_1,l_1}(M) \cap H_{\mathrm{sc}}^{m_2,l_2}(M) \to H_{\mathrm{sc}}^{m,l}(M) \tag{8.3}$$

where the left-hand side of (8.3) *is endowed with norm* $(\|\cdot\|^2_{m_1,l_1} + \|\cdot\|^2_{m_2,l_2})^{1/2}$.

The sc and qsc Sobolev space do provide comparable filtrations of $\mathcal{C}^{-\infty}(M)$:

Proposition 8.6. *For* $m \in \mathbb{Z}_+$,

$$H^{m,l}_{qsc}(M) \subset H^{m,l}_{sc}(M) \tag{8.4}$$

and

$$H^{0,m+l}_{sc}(M) \cap H^{m,l}_{sc}(M) \subset H^{m,l}_{qsc}(M) \tag{8.5}$$

The proof relies on Lemma 8.5 and the observation that

$$x^{-2l}(\kappa + \Delta)^m$$

(where κ is a positive constant) is an elliptic element of $\Psi^{2m,-2l}_{sc}(M)$ and a (non-elliptic) element of $\Psi^{2m,-2l}_{qsc}(M)$, while

$$x^{-2l}\left(\kappa x^{-2} + \Delta\right)^m$$

is an elliptic element of $\Psi^{2m,-2l}_{qsc}(M)$ and an element of

$$\Psi^{0,-2m-2l}_{scc}(M) + \Psi^{2,-2m-2l+2}_{scc}(M) + \cdots + \Psi^{2m,-2l}_{scc}(M).$$

9. Wavefront sets

Associated with our calculi of pseudodifferential operators is a notion of wavefront set, measuring microlocal regularity of distributions. As before, $*$ stands for sc(c) or qsc.

Definition 9.1. The (scattering/quadratic-scattering) wavefront set is the subset of C_*M such that $p \notin \mathrm{WF}_* u$ if and only if there exists $A \in \Psi^{0,0}_*(M)$ with $p \in \operatorname{ell} A$ such that $Au \in \dot{\mathcal{C}}^\infty(M)$.

There are also Sobolev versions of these wavefront sets: $p \in C_*M \notin \mathrm{WF}^{m,l}_* u$ if and only if there exists $A \in \Psi^{m,l}_*(M)$ with $p \in \operatorname{ell} A$ such that $Au \in L^2(M)$.

(As usual, we could have used operators of any order in the definition of $\mathrm{WF}_* u$.)

Both the sc and the qsc calculi reduce to the ordinary calculus of pseudodifferential operators when cut off away from ∂M, so the relevant wavefront sets generalize the traditional wavefront set introduced by Hörmander:

Proposition 9.2.

$$\mathrm{WF}_{sc} u \cap ({}^{sc}S^*M)^\circ = \mathrm{WF}_{qsc} u \cap ({}^{qsc}S^*M)^\circ = \mathrm{WF} u.$$

Example 9.3. Let $\phi(y)$ be a smooth function on ∂M. Then

$$\mathrm{WF}_{sc} e^{i\phi(y)/x} = \operatorname{graph}\left[d\left(\frac{\phi(y)}{x}\right)\right] \subset {}^{sc}T^*_{\partial M}M,$$

$$\mathrm{WF}_{qsc} e^{i\phi(y)/x^2} = \operatorname{graph}\left[d\left(\frac{\phi(y)}{x^2}\right)\right] \subset {}^{qsc}T^*_{\partial M}M.$$

On the other hand, $\mathrm{WF}_{\mathrm{qsc}} e^{i\phi(y)/x}$ lies in the zero section of ${}^{\mathrm{qsc}}\overline{T}^*M$ and $\mathrm{WF}_{\mathrm{sc}} e^{i\phi(y)/x^2}$ lies in the corner of ${}^{\mathrm{sc}}\overline{T}^*M$.

The function $e^{i\phi(y)/x}$ is an example of the "Legendre distributions" considered in [18].

The following proposition suggests that, morally speaking, the qsc wavefront set over ∂M is a "blowup" of the sc wavefront set in ${}^{\mathrm{sc}}S^*_{\partial M}M$. It will not be used in the sequel.

Proposition 9.4. *If* $u \in \mathcal{C}^\infty(M)$ *and*

$$\mathrm{WF}_{\mathrm{sc}} u \cap {}^{\mathrm{sc}}S^*_{\partial M}M = \emptyset,$$

then $\mathrm{WF}_{\mathrm{qsc}} u \subset 0$*, where* 0 *denotes the zero section of* ${}^{\mathrm{qsc}}\overline{T}^*_{\partial M}(M)$.

Proof. By localization, it suffices to prove the result for $M = S^n_+ = \mathrm{RC}(\mathbb{R}^n)$. We thus have coordinates near ∂M given by $\omega = z/|z| \in S^{n-1}$ and $x = |z|^{-1}$. Without loss of generality, assume $u \in \mathcal{C}^\infty(M)$ vanishes away from a small neighborhood of ∂M, so that these coordinates are valid on the support of $u = u(x, \omega)$.

Let M_q have defining function $\rho = x^2$; letting $\mathcal{F}_q$ denote Fourier transform on M_q (identified with $\mathbb{R}^n$ by RC^{-1}), we have

$$\begin{aligned}\mathcal{F}_q u(\eta) &= \int u(\sqrt{\rho}, \omega) e^{-i\omega\cdot\eta/\rho} \rho^{-n+1} d\rho d\omega \\ &= 2\int u(x, \omega) e^{-i\omega\cdot\eta/x^2} x^{-2n+3} dx d\omega.\end{aligned}$$

To conclude that $\mathrm{WF}_{\mathrm{qsc}} u \subset 0$, it suffices to show that

$$(1 - \phi(\eta)) \int u(x, \omega) e^{-i\omega\cdot\eta/x^2} x^{-2n+3} dx d\omega \in \mathcal{S}(\mathbb{R}^n_\eta)$$

if $\phi \in \mathcal{C}^\infty_c$ equals 1 on a neighborhood of the origin, as $\mathcal{F}_q^{-1}(1-\phi)\mathcal{F}_q \in \Psi_{\mathrm{qsc}}$ is elliptic on an arbitrary subset of ${}^{\mathrm{qsc}}\overline{T}^*_{\partial M}(M)\backslash 0$.

A calculation in Euclidian coordinates gives

$$\Delta e^{-i\omega\cdot\eta/x^2} = \sum_j D^2_{z_j} e^{-i(z\cdot\eta)|z|} = e^{-i\omega\cdot\eta/x^2} r(x, \omega, \eta)$$

where

$$r(x, \omega, \eta) = \left(-\frac{2(\eta\cdot\omega)}{i} + \frac{3(\eta\cdot\omega)^2}{x^2} + \frac{|\eta|^2}{x^2} \right).$$

Note that $|r(x, \omega, \eta)| \geqslant |\eta|^2/x^2$, so that on $\mathrm{supp}(1-\phi(\eta))$,

$$e^{-i\omega\cdot\eta/x^2} = \frac{1}{r(x, \omega, \eta)} \Delta e^{-i\omega\cdot\eta/x^2}. \tag{9.1}$$

Now we can apply the usual trick of integration by parts. We have

$$
\begin{aligned}
(9.2)\quad D_\eta^\alpha \int u(x,\omega)e^{-i\omega\cdot\eta/x^2}x^{-2n+3}dxd\omega \\
&= \int u(x,\omega)\frac{(-\omega)^\alpha}{x^{2|\alpha|}}e^{-i\omega\cdot\eta/x^2}x^{-2n+3}dxd\omega \\
&= \int u(x,\omega)(-\omega)^\alpha x^{-2n+3-2|\alpha|}\left(\frac{1}{r(x,\omega,\eta)}\Delta\right)^k e^{-i\omega\cdot\eta/x^2}dxd\omega
\end{aligned}
$$

for any $k \in \mathbb{Z}^+$ by (9.1). Our assumption on u is just that $u \in H_{sc}^{-\infty,l}(M)$ for some l. Thus, since $\Delta \in \Psi_{scc}^{2,0}(M)$, we have $\Delta^k u \in H_{sc}^{-\infty,l}(M)$ for all $k \in \mathbb{Z}^+$. This allows us to integrate by parts in (9.2). Since $r > |\eta|^2/x^2$, we find that (9.2) is rapidly-decreasing in η for any multi-index α. □

For our operators with parameter, there is a corresponding notion of wavefront set.

Definition 9.5. Let $u \in \mathcal{C}(\mathbb{R};\mathcal{C}^{-\infty}(M))$. For $S \subset \mathbb{R}$ compact, we say that $p \notin WF_*^S(u)$ if there exists a smooth family $A(t) \in \Psi_*^{0,0}(M)$ such that $A(t)$ is elliptic at p for all $t \in S$ and $Au \in \mathcal{C}(S;\dot{\mathcal{C}}^\infty(M))$.

There is a corresponding notion of Sobolev wavefront set.

Remarks.

1. It is perfectly possible to have $u \in \mathcal{C}(\mathbb{R};\mathcal{C}^{-\infty}(M))$ and $p \in S^*M$ with $p \in WF^S(u)$ but $p \notin WF(u(t))$ for any $t \in S$. A particularly germane example is given by the fundamental solution (1.2) to the free-particle Schrödinger equation on $\mathbb{R}$: take $u = (2\pi i t)^{-\frac{1}{2}}e^{iz^2/2t}$ on $\mathbb{R}_t \times \mathbb{R}_z$ (with $u = \delta(z)$ at $t = 0$). Let $S = [-1,1]$. Then $WF(u(t))$ is nonzero only for $t = 0$, at which time it is just $(0, \pm 1)$. On the other hand there must be points in $WF^S(u)$ over every point in $\mathbb{R}_z$, since otherwise we would have uniform estimates on $u(t)$ for $t \in S$ and z in some interval.
2. The scattering wavefront set is closely related to the "frequency set" used in semi-classical analysis; see [18], §11.

10. The Schrödinger equation

Given a self-adjoint operator $\mathcal{H} = \frac{1}{2}\Delta + V$, with $V \in \mathrm{Diff}_{qsc}^{1,1}(M)$ (and with Δ the Laplace-Beltrami operator for the metric g), we are interested in the Cauchy problem for the time-dependent Schrödinger equation

$$
\begin{aligned}
(D_t + \frac{1}{2}\Delta + V)\psi = 0, \\
\psi(0) = \psi_0 \in \mathcal{C}^{-\infty}(M).
\end{aligned}
\tag{10.1}
$$

Note that $\mathcal{H} \in \Psi_{qsc}^{2,0}(M)$, with $j_{qsc,2,0}(\mathcal{H}) = \frac{1}{2}j_{qsc,2,0}(\Delta)$.

Let $K_t = e^{-it\mathcal{H}}$ be the solution operator to (10.1). The spectral theorem guarantees that K_t exists as a unitary operator $L^2(M) \to L^2(M)$ for all t. Craig [3] uses energy conservation and a global commutator argument to obtain regularity of K_t in weighted Sobolev spaces. His arguments carry through, mutatis mutandis, in our setting. A consequence of Théorème 14 of [3] is that for $m \in \mathbb{Z}_+$,

$$K_t \in L^\infty_{loc}\left[\mathbb{R}_t; \mathcal{B}(H^{m,0}_{sc}(M) \cap H^{m-1,1}_{sc}(M) \cap \cdots \cap H^{0,m}_{sc}(M))\right];$$

in particular, we have $K_t : \dot{\mathcal{C}}^\infty(M) \to \dot{\mathcal{C}}^\infty(M)$ and, dually, $\mathcal{C}^{-\infty}(M) \to \mathcal{C}^{-\infty}(M)$. By Proposition 8.6 and Lemma 8.5, we thus have

$$K_t \in L^\infty_{loc}\left[\mathbb{R}_t; \mathcal{B}(H^{m,0}_{qsc}(M) \cap H^{0,m}_{qsc}(M), H^{m,0}_{qsc}(M))\right], \quad m \in \mathbb{Z}_+.$$

Since for $m > 0$,

$$H^{m,m}_{qsc}(M) \subset H^{m,0}_{qsc}(M) \cap H^{0,m}_{qsc}(M),$$

we obtain by duality

$$K_t \in L^\infty_{loc}\left[\mathbb{R}_t; \mathcal{B}(H^{-m,0}_{qsc}(M), H^{-m,-m}_{qsc}(M))\right], \quad m \in \mathbb{Z}_+. \tag{10.2}$$

Since $\cup_m H^{-m,0}_{qsc}(M) = \mathcal{C}^{-\infty}(M)$, (10.2) applies (for some m) to any $\psi_0 \in \mathcal{C}^{-\infty}(M)$.

Lemma 10.1. *Let* ψ *be the solution to* (10.1) *with* $\psi_0 \in \dot{\mathcal{C}}^\infty(M)$. *For any* $A(t) \in \Psi_{qsc}(M)$ *and* $t > 0$,

$$\langle A\psi, \psi\rangle|_0^T = \int_0^T \langle(\partial_t A + i[\mathcal{H}, A])\psi, \psi\rangle dt. \tag{10.3}$$

Proof. We compute

$$\begin{aligned} \partial_t\langle A\psi, \psi\rangle &= \left\langle \dot{A}\psi, \psi\right\rangle + \left\langle A\dot{\psi}, \psi\right\rangle + \left\langle A\psi, \dot{\psi}\right\rangle \\ &= \left\langle \dot{A}\psi, \psi\right\rangle + \langle -iA\mathcal{H}\psi, \psi\rangle + \langle A\psi, -i\mathcal{H}\psi\rangle \\ &= \left\langle \dot{A}\psi, \psi\right\rangle - i\langle A\mathcal{H}\psi, \psi\rangle + i\langle \mathcal{H}A\psi, \psi\rangle \\ &= \langle(\partial_t A + i[\mathcal{H}, A])\psi, \psi\rangle. \end{aligned} \tag{10.4}$$

Now integrate. □

(The identity (10.4) is extremely well-known, and can be found in virtually any quantum-mechanics text.)

Note that if $A \in \Psi^{m,l}_{qsc}(M)$ then $(\partial_t A + i[\mathcal{H}, A]) \in \Psi^{m+1,l+1}_{qsc}(M)$, and

$$j_{qsc,m+1,l+1}(\partial_t A + i[\mathcal{H}, A]) = (\partial_t + X)(j_{qsc,m,l}(A)),$$

where X is the Hamilton vector field of $\mathcal{H}$ (we study X in detail in Section 11).

Lemma 10.1 shows that if we make $(\partial_t A + i[\mathcal{H}, A])$ a negative operator (modulo lower-order terms), elliptic in some set, we can control

$$\langle A\psi(T), \psi(T)\rangle \text{ and } \int_0^T |\langle(\partial_t A + i[\mathcal{H}, A])\rangle| dt$$

in terms of $\langle A\psi(0), \psi(0)\rangle$, and obtain information about microlocal regularity of $\psi(T)$ in terms of microlocal regularity of $\psi(0)$. This is the argument used in §14.

11. Bicharacteristic flow

We now study the bicharacteristic flow for $\mathcal{H}$ on ${}^{\text{qsc}}\overline{T}^*M$. Let $\lambda dx/x^3 + \mu \cdot dy/x^2$ denote the canonical one-form on ${}^{\text{qsc}}\overline{T}^*M$, hence the symplectic form is

$$\omega = \frac{d\lambda \wedge dx}{x^3} + \frac{d\mu \wedge dy}{x^2} - 2\mu \frac{dx \wedge dy}{x^3}.$$

By (6.6),

$$j_{\text{qsc},2,0}(\mathcal{H}) = \frac{1}{2x^2}\left(\lambda^2 + |\mu|^2 + xr(\lambda, \mu)\right)$$

where r satisfies (6.5) (since V has order $(1,1)$, it does not contribute to the principal symbol). The Hamilton vector field of $j_{\text{qsc},2,0}(\mathcal{H})$ is given by

$$-\omega(X, \cdot) = d\left[\frac{1}{2x^2}\left(\lambda^2 + |\mu|^2 + xr(\lambda, \mu)\right)\right].$$

We split X into two pieces

$$X = \tilde{X} + P$$

where

$$\tilde{X} = \lambda x \partial_x + (\lambda^2 - |\mu|^2)\partial_\lambda + \langle \mu, \partial_y \rangle + 2\lambda\mu \cdot \partial_\mu - \frac{1}{2}\partial_y |\mu|^2 \cdot \partial_\mu \tag{11.1}$$

is the Hamilton vector field for the symbol $\frac{1}{2}x^{-2}(\lambda^2 + |\mu|^2)$, and

$$P = p_1 x^2 \partial_x + p_2 x \partial_y + q_1 x \partial_\lambda + q_2 x \partial_\mu \tag{11.2}$$

is the Hamilton vector field for the error term $\frac{1}{2}x^{-1}r(\lambda, \mu)$. (We distinguish different inner products by writing $\langle a, b\rangle = \sum a_i b_j \bar{h}^{ij}(y)$, and $a \cdot b = \sum a_i b_i$; $|\mu| = \langle \mu, \mu\rangle^{\frac{1}{2}}$ denotes the norm with respect to $\bar{h}$.) The functions p_1 and p_2 in (11.2) are smooth in x, y and are polynomials of degree one in λ, μ. The functions q_1 and q_2 are smooth in x, y and are polynomials of degree two in λ, μ. There are a number of conditions on the p's and q's stemming from the condition (6.5) on the error term $r(\lambda, \mu)$; the only one we shall need below is that

$$q_2 \in \lambda^2 x \mathcal{C}^\infty(x, y) + \lambda\mu\mathcal{C}^\infty(x, y) + \mu^2 \mathcal{C}^\infty(x, y). \tag{11.3}$$

We will treat P as a perturbation to $\tilde{X}$ near $x = 0$. Thus, we begin by analyzing the flow of the vector field $\tilde{X}$. Let t be the time-parameter for the flow. Away from $\{\mu = 0\}$

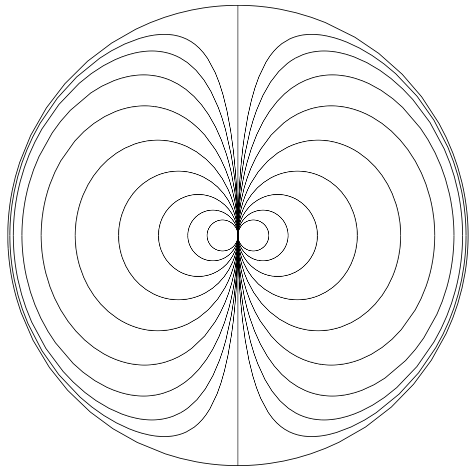

FIGURE 3. Integral curves of $\tilde{X}$, projected onto the (λ, μ) plane and radially compactified. The vertical line is the solution $\mu = 0$.

we follow [18] by introducing coordinates $\hat{\mu} = \mu/|\mu| \in S^{n-2}$ and reparametrizing, setting $ds/dt = |\mu|$. Then the flow along $\tilde{X}$ is given by

$$\frac{dy_i}{ds} = \bar{h}^{ij}\hat{\mu}_j \qquad \frac{d\hat{\mu}_i}{ds} = -\frac{1}{2}\hat{\mu}_j\hat{\mu}_k\partial_{y_i}\bar{h}^{jk} \tag{11.4}$$

$$\frac{d\lambda}{ds} = \frac{\lambda^2 - |\mu|^2}{|\mu|} \qquad \frac{d|\mu|}{ds} = 2\lambda \tag{11.5}$$

$$\frac{dx}{ds} = \frac{\lambda x}{|\mu|}. \tag{11.6}$$

Projecting onto the variables $(y, \hat{\mu})$ gives geodesic flow in the cosphere bundle of ∂M. Equation (11.5) also forms an autonomous system, which we can solve as follows: set $\alpha = \lambda/|\mu|$ to obtain the Riccati equation

$$\frac{d\alpha}{ds} = -1 - \alpha^2;$$

this has solution $\alpha = \tan(\theta - s)$; then

$$|\mu| = A\cos^2(\theta - s), \tag{11.7}$$

$$\lambda = \frac{A}{2}\sin 2(\theta - s) \tag{11.8}$$

and

$$x = C\cos^2(\theta - s).$$

The curves (11.7), (11.8) are shown in the radially compactified (λ, μ) plane in Figure 3.

Let $p = (x_0, y_0, \lambda_0, \mu_0)$ and let

$$(x(t), y(t), \lambda(t), \mu(t)) = \exp(t\tilde{X})[p]$$

be the result of flowing along $\tilde{X}$ starting at p for time t. Then $\theta = \arctan(\lambda_0/|\mu_0|)$, and $A = \mu_0 + \lambda_0^2/\mu_0$ (we take $\theta \in (-\pi/2, \pi/2)$). Since $t = \int \frac{ds}{|\mu|}$, we have $s - \theta \to \pm\pi/2$ as $t \to \pm\infty$. Thus, in terms of geodesic flow for $\bar{h}$,

$$Y_{\pm\infty}(p) = \exp_{y_0}^{(\bar{h})}\left(\theta \pm \frac{\pi}{2}\right)\hat{\mu}_0 = \lim_{t\to\pm\infty} y(t) \in \partial M.$$

If $\lambda_0 < 0$ then $\arctan(\lambda_0/|\mu_0|) + \pi/2 = -\arctan(|\mu_0|/\lambda_0)$, hence for $\lambda_0 < 0$,

$$Y_{+\infty}(p) = \exp_{y_0}\left(-\arctan(|\mu_0|/\lambda_0)\hat{\mu}_0\right).$$

Since $\frac{1}{u}\arctan u$ is a smooth function of u^2, $\arctan(|\mu_0|/\lambda_0)\hat{\mu}_0$ is smooth in μ_0 and hence $Y_{+\infty}$ is a smooth function on $\{\lambda_0 < 0\}$. Similarly, $Y_{-\infty}$ is a smooth function on $\{\lambda_0 > 0\}$.

The integral curves of $\tilde{X}$ obtained above exist for all t. We have, however, omitted from discussion some special integral curves: the set $\{x = \mu = 0\}$ is invariant under $\tilde{X}$ (and hence under X, since $X|_{\partial M} = \tilde{X}|_{\partial M}$), and on this set, $d\lambda/dt = \lambda^2$, i.e.

$$\lambda = \frac{\lambda_0}{1 - \lambda_0 t}.$$

Thus if $\lambda_0 > 0$ then $\lambda \to +\infty$ as $t \uparrow \lambda_0^{-1}$. Put another way, the flow starting at $p \in \{x = \mu = 0\}$ reaches the corner ${}^{\text{qsc}}S^*_{\partial M}M$ in finite time λ_0^{-1}. This is shown in Figure 3, in which the integral curve with $\mu = 0$ appears as a vertical line. The rest of the integral curves, with $\mu \neq 0$, stay in the interior of ${}^{\text{qsc}}\overline{T}^*_{\partial M}M$.

As the points $x = \mu = 0$ are particularly important, we describe them as follows:

Definition 11.1. Let $\mathcal{N} \subset {}^{\text{qsc}}\overline{T}^*M$ be the set given in our coordinates by $\{x = \mu = 0\}$. Let $\mathcal{N}_\pm \subset \mathcal{N}$ be the subsets on which $\pm\lambda \geqslant 0$. Let $\mathcal{N}^c_\pm = \mathcal{N}_\pm \cap {}^{\text{qsc}}S^*M$. We refer to $\mathcal{N}$ as the "normal set," with $\mathcal{N}_+$ being the "incoming normal set" and $\mathcal{N}_-$ the "outgoing normal set."

Remarks.

1. The reason for the above terminology is as follows: under the flow of the vector field X a point with $\lambda > 0$ travels away from ∂M, i.e. *into* the interior (or finite region, if M was obtained as a compactification). The "c" in $\mathcal{N}^c_\pm$ stands for "corner."
2. The manifolds $\mathcal{N}^c_\pm$ are naturally isomorphic to ∂M via the projection map on ${}^{\text{qsc}}\overline{T}^*M$.
3. The definition of $\mathcal{N}$ does depend on our choice of boundary defining function x. This is not a matter for concern, as the choice of a scattering metric g gives a distinguished boundary defining function up to second-order at ∂M (see [16] §6.1), so that $\mathcal{N}$ is well-defined given g.

Since $X = \tilde{X}$ on ${}^{\text{qsc}}\overline{T}^*_{\partial M}M$, the above description of the flow of $\tilde{X}$ applies to the perturbed vector field X, restricted to $x = 0$. We can thus regard $Y_{\pm\infty}$ as defined on

${}^{\mathrm{qsc}}\overline{T}^*_{\partial M}M$. We now need to extend this definition to (most of) the rest of ${}^{\mathrm{qsc}}\overline{T}^*M$. This is similar to the construction of "scattering coordinates" performed in [4].

As $\tilde{X}$ is homogeneous of degree one in λ, μ, it is natural to introduce new coordinates $\sigma = (\lambda^2 + |\mu|^2)^{-\frac{1}{2}}$, $\bar{\lambda} = \sigma\lambda$, $\bar{\mu} = \sigma\mu$, with $(\bar{\lambda}, \bar{\mu}) \in S^{n-1}$, and to study the vector field σX, which is homogeneous of degree zero. We have

$$\sigma\tilde{X} = \bar{\lambda}x\partial_x - |\bar{\mu}|^2\partial_{\bar{\lambda}} + \langle\bar{\mu}, \partial_y\rangle + \bar{\lambda}\bar{\mu}\cdot\partial_{\bar{\mu}} - \frac{1}{2}\partial_y|\bar{\mu}|^2\cdot\partial_{\bar{\mu}} - \bar{\lambda}\sigma\partial_\sigma. \tag{11.9}$$

The vector field σP is x times a smooth vector field, homogeneous of degree zero in $(\bar{\lambda}, \bar{\mu})$. Furthermore, since $\partial\bar{\mu}/\partial y$ and $\partial\bar{\mu}/\partial\lambda$ vanish at $\bar{\mu} = 0$, the coefficient of $\partial_{\bar{\mu}_i}$ in σP is given near $x = \bar{\mu} = 0$ by

$$x\sigma(q_2)_j\frac{\partial\bar{\mu}_i}{\partial\mu_j} + O(x\bar{\mu}). \tag{11.10}$$

Our restrictions (11.3) on the ∂_μ term in P can be written

$$q_2 = \sigma^{-2}\left((1 - |\bar{\mu}|^2)x\,\mathcal{C}^\infty(x,y) + \bar{\mu}(1 - |\bar{\mu}|^2)^{\frac{1}{2}}\,\mathcal{C}^\infty(x,y) + \bar{\mu}^2\,\mathcal{C}^\infty(x,y)\right).$$

Since $\partial\bar{\mu}_i/\partial\mu_j = \sigma(\delta_{ij} + O(\bar{\mu}^2))$, (11.10) is just $O(x^2) + O(x\bar{\mu})$ at $x = \bar{\mu} = 0$. The upshot is the following lemma, which is crucial for the conjugation argument we use later on.

Lemma 11.2. *The linear part of* $\sigma P(\bar{\mu})$ *vanishes at* $x = \bar{\mu} = 0$.

A vector field that is homogeneous of degree zero in σ pushes forward under the quotient to give a vector field on ${}^{\mathrm{qsc}}S^*M \cong {}^{\mathrm{qsc}}T^*M/\mathbb{R}^+$. Let X_S, $\tilde{X}_S$, P_S denote the vector fields obtained in this way from σX, $\sigma\tilde{X}$, and σP. (In our local coordinates, the quotient operation corresponds to dropping ∂_σ terms.)

Proposition 11.3. *In coordinates* $(x, y, \bar{\mu})$*, the linear part of* X_S *in* $(x, \bar{\mu})$ *near* $\mathcal{N}^c_\pm \subset {}^{\mathrm{qsc}}S^*M$ *is*

$$\pm x\partial_x \pm \bar{\mu}\cdot\partial_{\bar{\mu}} + \langle\bar{\mu}, \partial_y\rangle + xf(y)\cdot\partial_y$$

with $f_i(y) \in \mathcal{C}^\infty(\partial M)$ *for all* i.

Proof. In coordinates $(x, y, \bar{\mu})$ near $\bar{\lambda} = \pm 1$,

$$\tilde{X}_S = \bar{\lambda}x\partial_x - |\bar{\mu}|^2\partial_{\bar{\lambda}} + \langle\bar{\mu}, \partial_y\rangle + \bar{\lambda}\bar{\mu}\cdot\partial_{\bar{\mu}} - \frac{1}{2}\partial_y|\bar{\mu}|^2\cdot\partial_{\bar{\mu}}$$

with $\bar{\lambda} = \pm(1 - |\bar{\mu}|^2)^{\frac{1}{2}}$. Linearizing gives

$$\pm x\partial_x \pm \bar{\mu}\cdot\partial_{\bar{\mu}} + \langle\bar{\mu}, \partial_y\rangle.$$

Equation (11.2) shows that the coefficient of ∂_x in P_S is $O(x^2)$ and the coefficient of ∂_y is $O(x)$. Lemma 11.2 shows that the coefficient of $\partial_{\bar{\mu}}$ vanishes to second order in $(x, \bar{\mu})$ at $x = \bar{\mu} = 0$. So the only term in P_S contributing to the linearization of X_S is $O(x)\partial_y$. ∎

Among other things, Proposition 11.3 reveals that $\mathcal{N}_+^c$ is unstable and $\mathcal{N}_-^c$ stable under X_S.

We now investigate the long-time behavior of the flow of X_S.

Definition 11.4. A maximally extended integral curve of σX on ${}^{qsc}\overline{T}^*M$ is said to be *non-trapped forward/backward* if

$$\lim_{t\to\pm\infty} x(t) = 0.$$

A point not in $\mathcal{N}$ is said to be non-trapped forward/backward if the integral curve through it is non-trapped. A point in $\mathcal{N}\backslash 0$ with coordinates $(x = 0, y = y_0, \sigma = \sigma_0, \bar{\lambda} = \pm 1, \bar{\mu} = 0)$ in $\mathcal{N}_\pm$ is said to be non-trapped forward/backward if the point $(x = 0, y = y_0, \sigma = 0, \bar{\lambda} = \pm 1, \bar{\mu} = 0) \in \mathcal{N}_\pm^c$ is not in the closure of any forward-/backward-trapped integral curves.

Let $\mathcal{T}_\pm$ denote the set of forward-/backward-trapped points in ${}^{qsc}\overline{T}^*M$.

Definition 11.5. Let

$$N_{\pm\infty} : {}^{qsc}S^*M\backslash(\mathcal{N}_\pm^c \cup \mathcal{T}_\pm) \to \mathcal{N}_\mp^c$$

be given by

$$p \mapsto \lim_{t\to\pm\infty} \exp(t\sigma X)[p].$$

Let

$$Y_{\pm\infty} : {}^{qsc}\overline{T}^*M\backslash(\mathcal{N}_\pm \cup \mathcal{T}_\pm) \to \partial M$$

be given by

$$p \mapsto \lim_{t\to\pm\infty} \pi \exp(t\sigma X)[p],$$

where $\pi : {}^{qsc}\overline{T}^*M \to M$ is projection.

Theorem 11.6. *Let X be the bicharacteristic flow on ${}^{qsc}\overline{T}^*M$ corresponding to a Hamiltonian of the form*

(11.11)
$$\frac{1}{2x^2}\Big(\lambda^2 + |\mu|^2 + x r(\lambda,\mu)\Big); \quad r(\lambda,\mu) \in \lambda^2 x \mathcal{C}^\infty(x,y) + \lambda\mu\mathcal{C}^\infty(x,y) + \mu^2\mathcal{C}^\infty(x,y).$$

Then

(i) $N_{\pm\infty}$ *and* $Y_{\pm\infty}$ *are smooth maps.*

(ii) *If we let* $C_\pm^\epsilon$ *be the submanifold of* ${}^{qsc}S^*M$ *given by*

$$C_\pm^\epsilon = \Big\{x^2 + |\bar{\mu}|^2 = \epsilon, \bar{\lambda} \gtrless 0\Big\}$$

then for ϵ *sufficiently small,* $C_\mp^\epsilon$ *is a fibration over* ∂M *with projection map* $Y_{\pm\infty}$, *and every integral curve of* σX *which is not trapped forward/backward passes through* $C_\mp^\epsilon$*;*

(iii) *The sets* $\mathcal{T}_\pm\backslash\mathcal{N}_\pm^c$ *are closed subsets of* ${}^{qsc}S^*M\backslash\mathcal{N}_\pm^c$.

Remark. The class of Hamiltonians we allow is of course designed to include scattering metrics. On $\mathbb{R}^n$, it differs slightly from the principal symbols allowed in [4], which are not required to be polyhomogeneous at ∂M; the conditions on r in (11.11) are stronger than those of [4] in the λ^2 term and weaker (by an epsilon) in the other two terms.

Proof.

(i) Smoothness of $N_{\pm\infty}$ will follow from smoothness of $Y_{\pm\infty}$, as $Y_{\pm\infty} = \pi N_{\pm\infty}$. By homogeneity of σX, to show smoothness of $Y_{\pm\infty}$ it suffices to show that $Y_{\pm\infty}$ is smooth on ${}^{qsc}S^*M\backslash(\mathcal{N}_\pm \cup \mathcal{T}_\pm)$. As X_S is nonsingular except at $\mathcal{N}^c$ and is odd in the fiber variables, it suffices to prove that $Y_{+\infty}$ is smooth in a neighborhood of $\mathcal{N}_-^c$. Proposition 11.3 shows that in such a neighborhood,

$$X_S = -x\partial_x - \bar\mu \cdot \partial_{\bar\mu} + \langle \bar\mu, \partial_y \rangle + O(x)\partial_y + O(x^2 + \bar\mu^2).$$

By a linearization theorem of Sternberg [26] (or really a parametrized version of it, proven by Sell [22]) given any $y_0 \in \partial M$ we may replace $(x, \bar\mu)$ by smooth coordinates $(\tilde x, \tilde\mu)$ such that for y in a neighborhood of y_0 and $(x, \bar\mu)$ sufficiently small,

$$X_S = -\tilde x\partial_{\tilde x} - \tilde\mu \cdot \partial_{\tilde\mu} + \langle \tilde\mu, \partial_y \rangle + O(\tilde x)\partial_y + O(\tilde x^2 + \tilde\mu^2)\partial_y \tag{11.12}$$

with $(\tilde x, \tilde\mu) = (x, \bar\mu)$ to first order at $\mathcal{N}_-^c$. In other words, we can locally change coordinates so as to *linearize* the vector field in the $\tilde x$, $\tilde\mu$ variables.

In the region $\tilde x \neq 0$, set $\theta = \tilde\mu/\tilde x$, and use $(\tilde x, \theta, y)$ as coordinates. In this region, $d\tilde x/dt \neq 0$, so we can write the integral curves of X_S with $\tilde x$ as parameter:

$$\begin{aligned} \frac{dy_i}{d\tilde x} &= -\sum \bar h^{ij}(y)\theta_j + O(1) + O(\tilde x + \theta^2 \tilde x) \\ \frac{d\theta}{d\tilde x} &= 0. \end{aligned} \tag{11.13}$$

As $t \to \infty$, $x \to 0^+$, so $\lim_{t\to\infty} y$ is given by a finite-time solution to the ODE (11.13) (with θ considered to be a parameter) and hence is smooth in y_0, θ_0, and the initial point $\tilde x_0$.

At points in ${}^{qsc}S^*M\backslash\mathcal{N}_-^c$ where $\tilde x = 0$, we may without loss of generality take $\tilde\mu_1 \neq 0$. Now we set $\vartheta = (\tilde\mu_2, \dots, \tilde\mu_{n-1})/\tilde\mu_1$ and $\varpi = \tilde x/\tilde\mu_1$. Rewriting the flow with $\tilde\mu_1$ as parameter gives

$$\begin{aligned} \frac{dy_i}{d\tilde\mu_1} &= -\bar h^{i1}(y) + \sum_{j\neq 1} \bar h^{ij}(y)\vartheta_j + O(\varpi) + O(\tilde\mu_1\varpi^2 + \tilde\mu_1 + \tilde\mu_1\vartheta^2) \\ \frac{d\vartheta}{d\tilde\mu_1} &= \frac{d\varpi}{d\tilde\mu_1} = 0 \end{aligned} \tag{11.14}$$

As $t \to \infty$, $\tilde\mu \to 0^+$, so $\lim_{t\to\infty} y$ is given by a finite-time solution to the ODE (11.14) (with ϑ, ϖ considered as parameters) and hence is smooth in y_0, ϑ_0, ϖ_0, and the initial point $(\tilde\mu_1)_0$. This proves the smoothness of $Y_{\pm\infty}$.

(ii) By symmetry it suffices to prove that for sufficiently small ϵ, C_-^ϵ is a fibration over $\mathcal{N}_-^c$ and that every non-forward-trapped integral curve passes through it.

We can choose ϵ small enough that the set $\{x^2+|\bar{\mu}|^2 \leqslant 2\epsilon, \bar{\lambda} < 0\}$ is contained in a union of coordinate neighborhoods for ${}^{qsc}S^*M$ near $\partial({}^{qsc}S^*M)$ in which (11.12) holds and such that

$$2(\tilde{x}^2+|\tilde{\mu}|^2) > x^2+|\bar{\mu}|^2 > \frac{1}{2}(\tilde{x}^2+|\tilde{\mu}|^2) \tag{11.15}$$

on each of these neighborhoods (the $\tilde{x}$ and $\tilde{\mu}$ coordinates may be different on different neighborhoods). Every non-forward-trapped integral curve of X_S in ${}^{qsc}S^*M$ approaches $\mathcal{N}_-^c$ as $t \to \infty$, so to show that every non-forward-trapped integral curve passes through C_-^ϵ we need only show that every integral curve starting in $x^2+|\bar{\mu}|^2 < \epsilon$ passes through C_-^ϵ for some $t < 0$. Equation (11.12) shows that for any such curve,

$$\tilde{x}^2+\tilde{\mu}^2 = (\tilde{x}_0^2+\tilde{\mu}_0^2)e^{-2t}$$

(where $\tilde{\mu}^2 = \sum_i \tilde{\mu}_i^2$). As $\bar{h}^{ij}$ is bounded above and below, there must exist $c > 0$ such that

$$\tilde{x}^2+|\tilde{\mu}|^2 \geqslant c(\tilde{x}_0^2+|\tilde{\mu}_0|^2)e^{-2t} \text{ for } t < 0.$$

Thus by (11.15),

$$x^2+|\bar{\mu}|^2 \geqslant c'(x_0^2+|\bar{\mu}_0|^2)e^{-2t} \text{ for } t<0,\ x^2+|\bar{\mu}|^2 < 2\epsilon,$$

so every integral curve passes through C_-^ϵ.

To prove that $Y_{+\infty}$ gives a fibration of C_-^ϵ over ∂M, it suffices, by compactness of C_-^ϵ, to prove that $Y_{+\infty}$ is a submersion (see [13], III.5). We can check this locally in a coordinate patch, and separately on $C_-^\epsilon \cap \{\tilde{x} \neq 0\}$ and $C_-^\epsilon \cap \{\tilde{\mu}_i \neq 0\}$ (without loss of generality, take $i = 1$). Equation (11.13) in the former case, and (11.14) in the latter, now shows that $\partial Y_{+\infty}/\partial y$ is nonsingular.

(iii) Note that if $p \in ({}^{qsc}S^*M)\backslash(\mathcal{N}_\pm^c \cup \mathcal{T}_\pm)$, then there is a finite time $T \gtrless 0$ such that

$$\exp(TX_S)[p] \in \{x^2+|\bar{\mu}|^2 < \epsilon, \bar{\lambda} \lesseqgtr 0\},$$

where ϵ is chosen as in the construction of $C_\pm^\epsilon$ above. Since the flow is smooth for finite time, there is a neighborhood U of p such that

$$\exp(TX_S)[U] \subset \{x^2+|\bar{\mu}|^2 < \epsilon\}.$$

The linearization constructed above shows that $\mathcal{T}_\pm \cap \{x^2+|\bar{\mu}|^2 < \epsilon, \bar{\lambda} \lesseqgtr 0\} = \emptyset$, so that no point in U is trapped forward/backward, hence the complement of $\mathcal{T}_\pm$ is open.

□

In the case of $M = S_+^n = \mathrm{RC}(\mathbb{R}^n)$ with the Euclidian metric, the maps $Y_{\pm\infty}$ simply take a point $(z,\eta) \in S^*\mathbb{R}^n$ to the points $\pm\eta \in S^{n-1}$. If we perturb the Euclidean metric to an asymptotically Euclidian metric on $\mathbb{R}^n$, every geodesic in $\mathbb{R}^n$ has a limiting direction in S^{n-1} as $t \to \pm\infty$; these limiting directions are the values of $Y_{\pm\infty}$ in this more general case.

The flow of X_S in ${}^{qsc}S^*M$ leads us to consider the following "scattering relation" on $\mathcal{N}^c$.

Definition 11.7. Let $\mathcal{S} \subset \mathcal{N}^c_- \backslash \mathcal{T}_-$. The *scattering relation* on $\mathcal{S}$ is

$$\mathsf{Scat}(\mathcal{S}) = \mathsf{N}_{-\infty}\left(\mathsf{N}_{+\infty}^{-1}(\mathcal{S})\right) \subset \mathcal{N}^c_+.$$

In the example of $\mathbb{R}^n$ with an asymptotically Euclidian metric, the relation Scat takes a set of directions to all the directions which can "scatter into the set," i.e. all points in S^{n-1} which are asymptotic directions as $t \to -\infty$ of geodesics which asymptotically point in directions in $\mathcal{S}$ as $t \to +\infty$. If the metric is Euclidean, the scattering relation is particularly simple: $\pi(\mathsf{Scat}(\mathcal{S})) = -\pi(\mathcal{S})$ (where $-$ denotes the antipodal map).

Note that $\mathsf{Scat}(\mathcal{S})$ contains all the points in $\mathcal{N}^c_+$ that can be reached from $\mathcal{S}$ by geodesic flow at time π in ∂M. The time-π geodesic flow on the boundary was previously considered by Melrose and Zworski [18], who showed that the scattering matrix for a scattering metric is a Fourier integral operator associated to this relation. The relation Scat is more complicated, however, as it is affected by geodesics through the interior as well as those in the boundary.

Proposition 11.8. *The relation* Scat *takes closed sets to closed sets, and* Scat^{-1} *takes open sets to open sets.*

Proof. Let C^ϵ_- be chosen as in Theorem 11.6, so that every non-forward-trapped integral curve passes through it. Then

$$\mathsf{Scat} = \left(\mathsf{N}_{-\infty}|_{C^\epsilon_-}\right) \circ \left(\mathsf{N}_{+\infty}|_{C^\epsilon_-}\right)^{-1};$$

i.e. $\mathsf{Scat} = \Upsilon \circ \Xi^{-1}$, where Υ and Ξ are smooth with compact domain.

Let F be a closed set in $\mathcal{N}^c_-$. Then by continuity of Ξ, $\Xi^{-1}F$ is closed, and hence by compactness of C^ϵ_-, compact. Hence by continuity of Υ, $\mathsf{Scat}\, F$ is closed.

Let O be an open set in $\mathcal{N}^c_+$. Let $\mathsf{Scat}^{-1}(O) = \{p : \mathsf{Scat}(p) \subset O\}$. Then

$$(\mathsf{Scat}^{-1}(O))^c = \Xi\left[(\Upsilon^{-1}(O))^c\right]$$

By compactness of C^ϵ_-, $\left(\Upsilon^{-1}(O)\right)^c$ is compact, so that by continuity of Ξ, $(\mathsf{Scat}^{-1}(O))^c$ is compact as well. Hence $\mathsf{Scat}^{-1}(O)$ is open. □

12. The main theorems

We are now in a position to state the main theorems of this paper. Morally speaking, we show that if we interpret the flow of X on ${}^{qsc}S^*M$ as geodesic flow at infinite speed, then the flow of X on $C_{qsc}M$ does indeed describe the propagation of qsc wavefront set for a solution ψ of (10.1).

Theorem 12.1 (Propagation over the boundary). *Let* $p \in ({}^{qsc}\overline{T}^*_{\partial M} M)^\circ$ *and assume*

$$\exp(TX)[p] \in ({}^{qsc}\overline{T}^*_{\partial M} M)^\circ.$$

Then $\exp(TX)[p] \notin \mathrm{WF}_{qsc}\psi(T)$ *iff* $p \notin \mathrm{WF}_{qsc}\psi(0)$.

Theorem 12.2 (Propagation into the interior).

1. *Let* $p \in {}^{qsc}S^*M \backslash \mathcal{N}^c_-$ *be non-backward-trapped and let* $T > 0$. *If* $\exp(-TX)[N_{-\infty}(p)] \notin \mathrm{WF}_{qsc}\psi(0)$ *then* $p \notin \mathrm{WF}^{[T-\delta,T+\delta]}_{qsc}\psi$ *for some* $\delta > 0$.
2. *Conversely, let* $q \in \mathcal{N}^c_+$. *If for some neighborhood* U *of* q *in* ${}^{qsc}S^*M$ *and some* $T > 0$, $\delta > 0$ *we have*

$$\mathrm{WF}^{[T-\delta,T+\delta]}_{qsc}\psi \cap (U \backslash \mathcal{N}^c_+) \cap N^{-1}_{-\infty}(q) = \emptyset$$

then $\exp(-TX)[q] \notin \mathrm{WF}_{qsc}\psi(0)$.

Theorem 12.3 (Propagation into the boundary).

1. *Let* $q \in \mathcal{N}^c_-$. *If for some neighborhood* U *of* q *in* ${}^{qsc}S^*M$ *and some* $\delta > 0$ *we have*

$$\mathrm{WF}^{[-\delta,\delta]}_{qsc}\psi \cap (U \backslash \mathcal{N}^c_-) \cap N^{-1}_{+\infty}(q) = \emptyset$$

then $\exp(TX)[q] \notin \mathrm{WF}_{qsc}\psi(T)$ *for all* $T > 0$.
2. *Conversely, let* $p \in {}^{qsc}S^*M \backslash \mathcal{N}^c_+$ *be non-forward-trapped. If* $\exp(TX)[N_{+\infty}(p)] \notin \mathrm{WF}_{qsc}\psi(T)$ *then* $p \notin \mathrm{WF}^{[-\delta,\delta]}_{qsc}\psi$ *for some* $\delta > 0$.

Theorem 12.4 (Scattering across the interior). *Let* $p \in \mathcal{N}_- \backslash \{0\}$ *have coordinates* $(x = 0, y = y_0, \lambda = -\lambda_0, \mu = 0)$. *Let* $q = \exp(-\lambda_0^{-1}X)[p] \in \mathcal{N}^c_-$. *If* q *is not backward-trapped and*

$$\exp(-(T - \lambda_0^{-1})X)\,[\mathsf{Scat}(q)] \cap \mathrm{WF}_{qsc}\psi(0) = \emptyset$$

for some $T > \lambda_0^{-1}$, *then* $p \notin \mathrm{WF}_{qsc}\psi(T)$.

Theorem 12.5 (Global propagation into the boundary). *Let* $p \in \mathcal{N}_- \backslash \{0\}$ *have coordinates* $(x = 0, y = y_0, \lambda = -\lambda_0, \mu = 0)$. *Let* $q = \exp(-\lambda_0^{-1}X)[p] \in \mathcal{N}^c_-$. *If* q *is not backward-trapped and*

$$\overline{N^{-1}_{+\infty}(q)} \cap \mathrm{WF}_{qsc}\psi(0) = \emptyset$$

(*closure taken in* ${}^{qsc}S^*M$) *then* $p \notin \mathrm{WF}_{qsc}\psi(\lambda_0^{-1})$.

Part 1 of Theorems 12.2 and 12.3 and Theorem 12.4 are illustrated in Figures 4–6. In these diagrams M is two-dimensional; this means that we can only draw one dimension of the fibers of ${}^{qsc}\overline{T}^*M$.

Remarks.

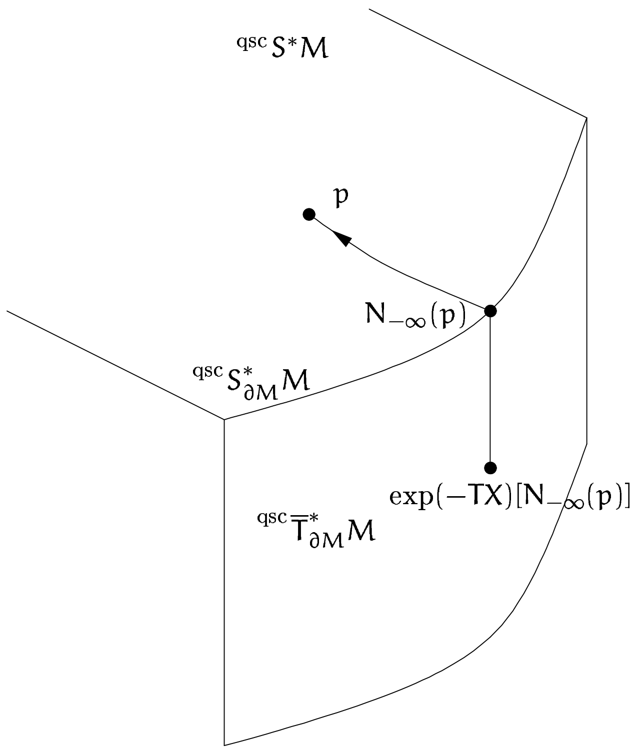

FIGURE 4. Theorem 12.2, Part 1.

1. As discussed in §11, if $p \in ({}^{\mathrm{qsc}}\overline{T}^*_{\partial M}M)^\circ \backslash \mathcal{N}_+$ then

$$\exp(TX)[p] \in \left({}^{\mathrm{qsc}}\overline{T}^*_{\partial M}M\right)^\circ \tag{12.1}$$

   for all $T > 0$; if $p \in \mathcal{N}_+$, then (12.1) holds for $T < \lambda(p)^{-1}$, hence Theorem 12.1 applies to such p, T. In Theorem 12.2, $\exp(-TX)[q]$ is defined for $q \in \mathcal{N}_+^c$ and $T > 0$: recall that the flow on $\mathcal{N}_+$ reaches the corner in finite (positive) time. Similarly, of course, $\exp(TX)[q]$ in Theorem 12.3 makes sense for $q \in \mathcal{N}_-^c$ and $T > 0$.
2. If there are no trapped rays, then given any $T > 0$ and any $p \in C_{\mathrm{qsc}}M$, Theorems 12.1, 12.2, 12.4, and 12.5 yield a set $\mathcal{G}_T(p) \subset ({}^{\mathrm{qsc}}\overline{T}^*_{\partial M}M)^\circ$ such that if $\mathrm{WF}_{\mathrm{qsc}}\psi(0) \cap \mathcal{G}_T(p) = \emptyset$, then $p \notin \mathrm{WF}_{\mathrm{qsc}}\psi(T)$. For $p \in {}^{\mathrm{qsc}}\overline{T}^*_{\partial M}M \backslash \mathcal{N}_-$, $\mathcal{G}_T(p)$ is a point in ${}^{\mathrm{qsc}}\overline{T}^*_{\partial M}M \backslash \mathcal{N}_-$. For $p \in {}^{\mathrm{qsc}}S^*M$, $\mathcal{G}_T(p)$ is a point in $\mathcal{N}_+$. For $p \in \mathcal{N}_-$, $\mathcal{G}_T(p)$ is either another point in $\mathcal{N}_-$ (for $T < -\lambda(p)^{-1}$), a set in ${}^{\mathrm{qsc}}S^*M$ (for $T = -\lambda(p)^{-1}$), or a set in $\mathcal{N}_+$ determined by the scattering relation (for $T > -\lambda(p)^{-1}$). In the absence of complications due to trapped rays, Theorems 12.1–12.5 are thus a complete propagation result for qsc wavefront set.
3. The observations made in the introduction about smoothness of solutions to the free Schrödinger equation on $\mathbb{R}^1$ can be recovered from Theorem 12.2: we use a

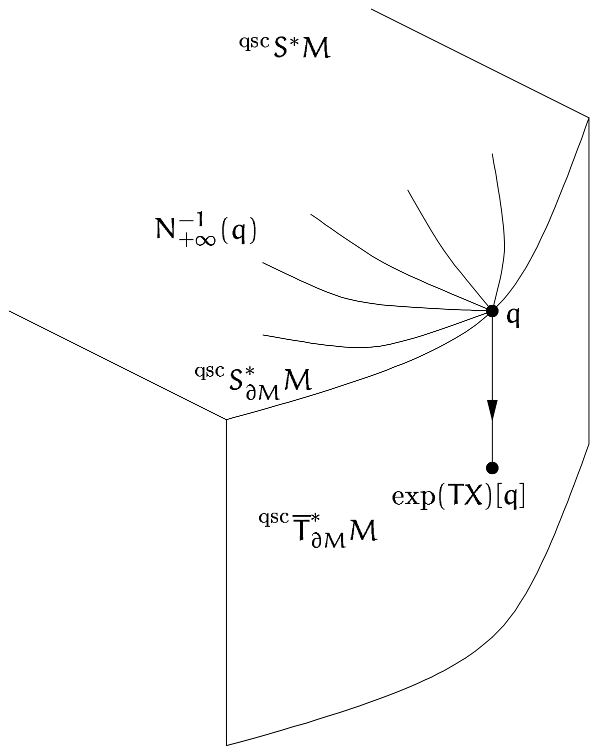

FIGURE 5. Theorem 12.3, Part 1.

boundary defining function x on S^1_+ given by $1/|z|$ near ∂S^1_+. Then $e^{-i\lambda z^2/2} = e^{-i\lambda/x^2}$. As observed in Example 9.3,

$$\mathrm{WF}_{\mathrm{qsc}} e^{-i\lambda/x^2} = \mathrm{graph}\,\lambda \frac{dx}{x^3},$$

and Theorem 12.2 predicts that this Cauchy data can only result in a singularity at time $t = \lambda^{-1}$.

4. One of the main results of Craig, Kappeler and Strauss [4] is that if $\psi(0)$ has no scattering wavefront set at an inward-pointing normal point in the corner of $C_{\mathrm{sc}}M$, then for *all* $t > 0$, $\psi(t)$ is microlocally smooth along geodesics emanating from that corner point. As we have seen in Proposition 9.4, qsc wavefront set is, loosely speaking, a blowup of the sc wavefront set in the corner. In fact the hypotheses used in [4] imply that $\mathrm{WF}_{\mathrm{qsc}}\psi(0) \cap (\mathcal{N}_+ \backslash 0) = \emptyset$, hence we can recover the microlocal smoothness result of [4] from Theorem 12.2. Note, however that significantly weaker hypotheses on V are allowed in [4] than in this paper.
5. The use of $\mathrm{WF}_{\mathrm{qsc}}^{[T-\delta,T+\delta]}$ in Theorem 12.2, Part 2 and of $\mathrm{WF}_{\mathrm{qsc}}^{[-\delta,\delta]}$ in Theorem 12.3, Part 1 is indispensable. The latter result, for example, is not true if we replace $\mathrm{WF}_{\mathrm{qsc}}^{[-\delta,\delta]}\psi$ with $\mathrm{WF}_{\mathrm{qsc}}\psi(0)$—see the remark in §9 following the definition of WF^S_*.

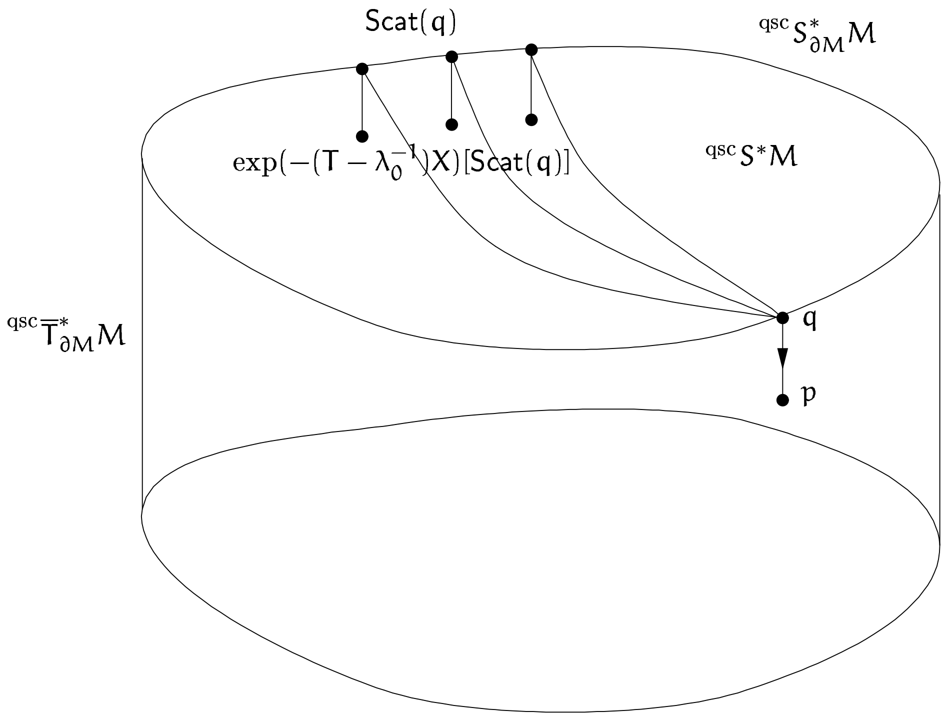

FIGURE 6. Theorem 12.4.

6. Theorems 12.3 and 12.2 are trivially equivalent owing to time-reversal symmetry: if $\psi(t)$ is a solution to (10.1) then so is $\overline{\psi(-t)}$. It will suffice to prove only the first part of each of these theorems.

The proofs of the above theorems will be deferred to §14. First, we must construct the symbols of the test operators used in the proofs.

13. SYMBOL CONSTRUCTION

As discussed in §10, we aim to find qsc-operators A such that

$$\partial_t A + i[\mathcal{H}, A] \tag{13.1}$$

has a symbol which is negative in regions in which we with to prove regularity. In order to avoid difficulties with Gårding inequalities, we will want (13.1) to be minus a sum of squares plus manageable error terms.

The casual reader may wish to skip ahead to §14, in which the constructions of this section are used to prove the main theorems, referring back to this section as necessary.

We will construct the following symbols:

1. a_∂ for propagation within $({}^{\text{qsc}}\overline{T}^*_{\partial M})^\circ$
2. a_+ and $\tilde{a}_+$ for propagation out of $({}^{\text{qsc}}\overline{T}^*_{\partial M})^\circ$ and into ${}^{\text{qsc}}S^*M$

3. $a_\circ$ and $\tilde{a}_\circ$ for propagation across ${}^{qsc}S^*M$
4. a_- and $\tilde{a}_-$ for propagation out of ${}^{qsc}S^*M$ and back into $\mathcal{N}_-$.

The symbols $\tilde{a}_+$, $\tilde{a}_\circ$, and $\tilde{a}_-$ are time-independent versions of a_+, $a_\circ$, and a_- required for the proof of Theorem 12.5.

First, we set some notation for the remainder of this section. Let H be the Heaviside step function. Let ϕ be a smooth, non-increasing function on $\mathbb{R}$ with

$$\phi(x) = \begin{cases} 1, & x < 1/2 \\ 0, & x > 1 \end{cases}$$

We will select a number of small constants ϵ_i later on; let $\phi_i(x) = \phi(x/\epsilon_i)$. Let $\chi(x)$ be a smooth, nondecreasing approximation to the Heaviside function

$$\chi(x) = \begin{cases} 0, & x < 0 \\ 1, & x > \epsilon_\chi \end{cases}$$

where $\epsilon_\chi > 0$ is a small constant. We may assume that ϕ, χ, $-\phi'(x)$, and $\chi'(x)$ are squares of smooth functions.

Construction of a_∂. This symbol is the simplest to construct, as we can more or less use the flowout of a bump-function. Given $p \in ({}^{qsc}\overline{T}^*_{\partial M}M)^\circ$, let ψ be a non-negative function on ${}^{qsc}\overline{T}^*M$ that is nonzero on a(n arbitrarily small) neighborhood of p; we may furthermore assume that ψ has a smooth square root. For $m, l \in \mathbb{R}$, set

$$a_\partial^{m,l}(t,q) = ((1+t)^\alpha x)^{l-m}\psi(\exp(-tX)[q])\phi_1(x) \in \mathcal{C}^\infty(\mathbb{R}_t; \mathcal{A}^{[+\infty,l-m]}(C_{qsc}M))$$

(this expression in local coordinates makes sense globally because of the presence of the cutoff $\phi_1(x)$). We use the supersript (m,l) on a_∂ because we will later think of a_∂ as the symbol of an element of $\Psi^{m,l}_{qsc}(M)$; a priori, though, it could be the symbol of an element of $\Psi^{m+k,l+k}_{qsc}(M)$ for any k. Note that a_∂ has a square root in $\mathcal{A}^{[+\infty,(l-m)/2]}({}^{qsc}\overline{T}^*M)$.

We now have

$$(-\partial_t - X)a_\partial^{m,l} = \left[-(l-m)\left(\frac{\alpha}{1+t} + \lambda\right) + O(x)\right] a_\partial^{m,l}$$

as an element of $\mathcal{A}^{[+\infty,l-m]}(C_{qsc}M)$ (we have suppressed the ϕ_1' term because it is supported away from $C_{qsc}M$). Given any T, we can choose $|\alpha|$ sufficiently large and $\operatorname{supp}\psi$ sufficiently small that $|\alpha/(1+t)| > |\lambda|$ on $\operatorname{supp} a_\partial$ for all $t \in [0,T]$; if we then choose the sign of α opposite to that of $l-m$ and ϵ_1 sufficiently small, then

$$(13.2) \qquad (-\partial_t - X)a_\partial^{m,l} = (c_\partial^{(m+1)/2,(l+1)/2})^2 \in \mathcal{A}^{[+\infty,l-m]}(C_{qsc}M) \quad \text{for } t \in [0,T],$$

with $c_\partial^{(m+1)/2,(l+1)/2} \in \mathcal{C}^\infty([0,T]; \mathcal{A}^{[+\infty,(l-m)/2]}(C_{qsc}M))$. (As the reader has probably divined, we will take $c_\partial^{(m+1)/2,(l+1)/2}$ to be the symbol of an element of an element of $\Psi^{(m+1)/2,(l+1)/2}_{qsc}(M)$.)

The salient features of a_∂ are the property (13.2), and the fact that

$$a_\partial(0) \neq 0 \text{ at } p,$$
$$a_\partial(T) \neq 0 \text{ at } \exp(TX)[p].$$

Construction of a_+ and $\tilde{a}_+$. This construction is trickier than that of a_∂ because X vanishes on $\mathcal{N}^c$, so standard constructions do not apply.

Let $p \in \mathcal{N}_+$ have coordinates $(x = 0, y = y_0, \lambda = \lambda_0, \mu = 0)$ (and hence $\sigma_0 = \lambda_0^{-1}$—recall that $\sigma = (\lambda^2 + |\mu|^2)^{-\frac{1}{2}}$). Set

$$b_+ = \chi(\sigma - \sigma_0 + \epsilon_2 + \alpha t)\chi(-\sigma + \sigma_0 + \epsilon_2 - \beta t)$$

where $\alpha < 1 < \beta$ and $\epsilon_2 > \epsilon_\chi$; we choose α and β sufficiently close to 1 that $b_+(t = \sigma_0, \sigma = 0) = 1$. The function b_+ is thus supported in a "window" moving toward $\sigma = 0$ and initially centered at σ_0, with its leading edge moving a bit more slowly than unit speed, and its trailing edge a bit faster. Hence

$$(-\partial_t - X)b_+ = (-\partial_t + (\bar{\lambda} + O(x))\partial_\sigma)b_+$$

is non-negative for $\bar{\lambda}$ close to 1. Thus if we choose ϵ_3 and ϵ_4 sufficiently small (the size of ϵ_4 is dictated by α and β) then $\phi_3(x)\phi_4(|\bar{\mu}|)(-\partial_t + \bar{\lambda}\partial_\sigma)b_+$ is a sum of squares of smooth functions.

We let $\psi_{-\infty}(p') = \phi_5(d(Y_{-\infty}(p'), y_0))$ where $d(\cdot,\cdot)$ is Riemannian distance in ∂M, and let

$$a_+^{m,l} = \sigma^{-m}x^{l-m}\psi_{-\infty}\phi_3(x)\phi_4(|\bar{\mu}|)b_+H(\bar{\lambda})$$

(note that the $H(\bar{\lambda})$ serves only to select one of the two components of the support of the smooth function that it multiplies). We have $X\psi_{-\infty} = 0$, since $Y_{-\infty}$ is constant along integral curves. $X\phi_3(x) = (\bar{\lambda} + O(x))\sigma^{-1}x\phi_3'(x)$, which is minus a square, when multiplied by b_+. Also

$$X\phi_4(|\bar{\mu}|) = \sigma^{-1}\left[\bar{\lambda}|\bar{\mu}| + O(|\bar{\mu}|^2) + O(x)\right]\phi_4'(|\bar{\mu}|),$$

so that if ϵ_3 and ϵ_4 are sufficiently small this function times $\phi_3(x)$ is minus a square. We further have

$$X(\sigma^{-m}x^{l-m}) = l\bar{\lambda}\sigma^{-m-1}x^{l-m} + O(\sigma^{-m-1}x^{l-m+1}). \tag{13.3}$$

By the foregoing observations, if $l < 0$ we can write

$$(-\partial_t - X)a_+^{m,l} = (c_+^{(m+1)/2,(l+1)/2})^2 + \sum_i d_i^2 \tag{13.4}$$

with

$$d_i, c_+ \in \mathcal{C}^\infty([0,T]; \mathcal{A}^{[(m+1)/2,(l+1)/2]}(C_{qsc}M))$$

and with c_+ nonzero where a_+ is. The point of this symbol construction is that, in addition to (13.4), we have

$$a_+(0) \neq 0 \text{ at } p,$$
$$a_+(\lambda_0^{-1}) \neq 0 \text{ at } \exp(\lambda_0^{-1}X)[p] \in \mathcal{N}_+^c.$$

We further set

$$\tilde{a}_+^{m,l} = \sigma^{-m}x^{l-m}\psi_{-\infty}b(\sigma)\phi_3(x)\phi_4(|\bar{\mu}|)H(\bar{\lambda})$$

where

$$b(\sigma) = \phi(\sigma/\epsilon_\sigma). \tag{13.5}$$

Thus it is not the case that $(-\partial_t - X)\tilde{a}_+$ is a sum of squares: there will be a negative term involving $Xb(\sigma)$, and we can write

$$(-\partial_t - X)\tilde{a}_+^{m,l} = (\tilde{c}_+^{(m+1)/2,(l+1)/2})^2 + \sum_i d_i^2 + g$$

where $\operatorname{supp} g$ is contained in an arbitrarily small neighborhood of a the single point $(y = y_0, \bar{\mu} = 0, \sigma = 0)$ in ${}^{qsc}\overline{T}^*_{\partial M}M$, and $\tilde{c}_+$ has the same properties as c_+ above.

Construction of $a_\circ$ and $\tilde{a}_\circ$. The construction is again more or less standard, as we stay away from $\mathcal{N}$, where X is singular; the only issue is the conormal singularity of X at the whole boundary face ${}^{qsc}S^*M$.

Suppose $p \in {}^{qsc}S^*M$ is not trapped backward. Then given any $\epsilon_x > 0$, $\epsilon_y > 0$, and $\epsilon_{\bar{\mu}} > 0$, there exists $K > 0$ such that

$$\exp(r\sigma X)[p] \in \{x < \epsilon_x, |\bar{\mu}| < \epsilon_{\bar{\mu}}, d(y, Y_{-\infty}(p)) < \epsilon_y\}$$

for $r < -K+1$. Since σX is nonsingular for $p \notin \mathcal{N}$, we can find coordinates $(w_1, \dots, w_{2n})$ on ${}^{qsc}\overline{T}^*M$, valid in a neighborhood containing both p and $\exp(-K\sigma X)[p]$, with $w \in \mathbb{R}^{2n-1} \times \mathbb{R}_+$ if $p \in ({}^{qsc}S^*M)^\circ$ or $w \in \mathbb{R}^{n-2} \times \mathbb{R}_+^2$ if p is in the corner, and such that $w(p) = 0$, $X = \partial_{w_1}$, $w_{2n} \in \sigma\mathcal{C}^\infty({}^{qsc}\overline{T}^*M)$ is a defining function for ${}^{qsc}S^*M$, and, in the corner case, $w_{2n-1} \in x\mathcal{C}^\infty({}^{qsc}\overline{T}^*M)$ is a defining function for ${}^{qsc}\overline{T}^*_{\partial M}M$.

If $p \in ({}^{qsc}S^*M)^\circ$, set

$$a_\circ^{m,l} = w_{2n}^{-m}(w_1 + K)\chi(w_1 + K)\chi(-w_1 + \epsilon_\chi)\chi(-w_1 - K + \frac{t}{\epsilon_t})\phi_5(|(w_2, \dots, w_{2n})|).$$

By choosing ϵ_5, we can keep $\sup \sigma$ as small as we like on $\operatorname{supp} \chi(w_1 + K)\chi(-w_1 + \epsilon_\chi)\phi_5(|(w_2, \dots, w_{2n})|)$ (since σ is bounded by a multiple of w_{2n}). We require $\epsilon_t > \sup \sigma$; thus

$$\begin{aligned}\chi(w_1 + K)\chi(-w_1 + \epsilon_\chi)\phi_5(|(w_2, \dots, w_{2n})|)(-\partial_t - X)\chi\left(-w_1 - K + \frac{t}{\epsilon_t}\right)\\ = \chi(w_1 + K)\chi(-w_1 + \epsilon_\chi)\phi_5(|(w_2, \dots, w_{2n})|)\chi'\left(w_1 + K - \frac{t}{\epsilon_t}\right)\left(\sigma^{-1} - \epsilon_t^{-1}\right)\end{aligned}$$

is the square of a smooth function.

Of the other terms in $(-\partial_t - X)a_\circ$, the only one that is not a square is that obtained by differentiating $\chi(w_1 + K)$. This term, however, has the virtue of being supported in $\{x < \epsilon_x, |\bar\mu| < \epsilon_{\bar\mu}, \sigma < \epsilon_5, d(y, Y_{-\infty}(p)) < \epsilon_y\}$. The term obtained by differentiating $(K + w_1)$ we denote $(c_\circ^{(m+1)/2,(l+1)/2})^2$; then $c_\circ$ is nonzero where $a_\circ$ is.

If $p \in {}^{qsc}S^*_{\partial M}M$, set

$$a_\circ^{m,l} = w_{2n}^{-m} w_{2n-1}^{l-m} (K + w_1)\chi(w_1 + K)\chi(-w_1 + \epsilon_\chi)\chi(-w_1 - K + \frac{t}{\epsilon_t})\phi_5(|(w_2, \dots, w_{2n})|);$$

the same observations apply as in the interior case.

In either case, $a_\circ(0) = 0$, $a_\circ \neq 0$ at p for $t > (w_1 + K)\epsilon_t$, and

$$(13.6)\quad (-\partial_t - X)a_\circ^{m,l} = (c_\circ^{(m+1)/2,l/2})^2 + \sum e_i^2 \\ + \text{ terms supported in } \{x < \epsilon_x, |\bar\mu| < \epsilon_{\bar\mu}, \sigma < \epsilon_5, d(y, Y_{-\infty}(p)) < \epsilon_y\}.$$

We also set

$$\tilde a_\circ^{m,l} = w_{2n}^{-m}(w_1 + K)\chi(w_1 + K)\chi(-w_1 + \epsilon_\chi)\phi_5(|(w_2, \dots, w_{2n})|)$$

if we have chosen a point $p \in ({}^{qsc}S^*M)^\circ$ and

$$\tilde a_\circ^{m,l} = w_{2n}^{-m} w_{2n-1}^{l-m}(K + w_1)\chi(w_1 + K)\chi(-w_1 + \epsilon_\chi)\phi_5(|(w_2, \dots, w_{2n})|)$$

if $p \in {}^{qsc}S^*_{\partial M}M$. As before, we have $\tilde a_\circ \neq 0$ at p and

$$(13.7)\quad (-\partial_t - X)\tilde a_\circ^{m,l} = (\tilde c_\circ^{(m+1)/2,l/2})^2 + \sum e_i^2 \\ + \text{ terms supported in } \{x < \epsilon_x, |\bar\mu| < \epsilon_{\bar\mu}, \sigma < \epsilon_5, d(y, Y_{-\infty}(p)) < \epsilon_y\}.$$

with $\tilde c_\circ$ nonzero where $\tilde a_\circ$ is.

Construction of a_- and $\tilde a_-$. Let $q \in \mathcal{N}^c_-$. Set $\psi_\infty(p') = \phi_6(d(Y_{+\infty}(p'), \pi(q)))$, $b_-(t) = \chi(-\sigma + \gamma t)$ with $\gamma < 1$, and

$$a_-^{m,l} = \sigma^{-m} x^{l-m} \psi_\infty b_- \phi_7(x)\phi_8(|\bar\mu|)H(-\bar\lambda).$$

If $l > 0$ then by (13.3), $(-\partial_t - X)a_-^{m,l}$ contains a term $(c_-^{(m+1)/2,(l+1)/2})^2$ with c_- nonzero where a_- is. The term in $(-\partial_t - X)a_-^{m,l}$ containing $(-\partial_t - X)b_-$ is a square provided ϵ_7 and ϵ_8 are sufficiently small. There are several non-positive terms in $(-\partial_t - X)a_-$ obtained from differentiating ϕ_7 and ϕ_8; these terms are supported in an arbitrarily small neighborhood of q, but away from $\mathcal{N}^c$.

We also set

$$\tilde a_-^{m,l} = \sigma^{-m} x^{l-m} \psi_\infty b(\sigma)\phi_7(x)\phi_8(|\bar\mu|)H(-\bar\lambda).$$

where $b(\sigma)$ is again defined by (13.5). Then

$$(-\partial_t - X)\tilde a_-^{m,l} = (\tilde c_-^{(m+1)/2,(l+1)/2})^2 + \sum_i d_i^2 + g$$

with $\tilde{c}_-$ nonzero where $\tilde{a}_-$ is and with $\operatorname{supp} g$ contained in an arbitrarily small neighborhood of the point q but away from $\mathcal{N}^c$.

14. Proof of the main theorems

Positive-commutator arguments of the type that we use in this section date back to Hörmander [8], who used similar arguments in the original proof of his theorem on propagation of singularities for operators of real principal type. Positive-commutator methods have recently been applied to the time-dependent Schrödinger equation by Sigal-Soffer [25] in the finite-energy setting, and by Craig, Kappeler, and Strauss [4]; further references on positive-commutator methods in scattering theory can be found in these two papers. The arguments employed in this section are modeled on those in [4].

Recall that we need only prove part one of each of Theorems 12.2 and 12.3: the remaining parts follow by time-reversal.

The Cauchy data $\psi(0)$ is in $H^{m_0,l_0}_{\mathrm{qsc}}(M)$ for some m_0, l_0. By (10.2),

$$K_t \in L^\infty_{\mathrm{loc}}\left[\mathbb{R}_t; \mathcal{B}(H^{m_0,l_0}_{\mathrm{qsc}}(M), H^{m,l}_{\mathrm{qsc}}(M))\right] \tag{14.1}$$

for some (m, l), i.e. there is a constant C such that

$$\|\psi(t)\|_{m,l} \leqslant C\|\psi(0)\|_{m_0,l_0}. \tag{14.2}$$

for all $t \in [0, T]$. Since $H^{p,q}_{\mathrm{qsc}}(M) \subset H^{p-k,q+k}_{\mathrm{qsc}}(M)$ and $H^{p,q}_{\mathrm{qsc}}(M) \subset H^{p,q-k}_{\mathrm{qsc}}(M)$ for all $k > 0$ and all p and q, we may assume that $l < 0$ or $l > 0$, as we please; we can also take $H^{m_0,l_0}_{\mathrm{qsc}}(M) \subset H^{m,l}_{\mathrm{qsc}}(M)$.

We will require smooth solutions to the Schrödinger equation in order to carry out commutator arguments. Thus, given $\psi(0) \in H^{m,l}_{\mathrm{qsc}}(M)$, let

$$\psi_n(0) = \operatorname{Op}\left((1 - \phi(nx))(1 - \phi(n\sigma))\right)\psi(0)$$

and

$$\psi_n(t) = K_t\psi_n(0).$$

Then $\psi_n(t) \in \dot{\mathcal{C}}^\infty(M)$ for all t, and by Proposition 7.1 and (14.1),

$$\psi_n \to \psi \text{ in } L^\infty([0, T]; H^{m,l}_{\mathrm{qsc}}(M)).$$

Proof of Theorem 12.1. Let $p \in ({}^{\mathrm{qsc}}\overline{T}^*_{\partial M}M)^\circ$ and assume

$$\exp(TX)[p] \in \left({}^{\mathrm{qsc}}\overline{T}^*_{\partial M}M\right)^\circ$$

and

$$p \notin \mathrm{WF}_{\mathrm{qsc}}\psi(0).$$

Construct $a^{2m,2l}_\partial$ as in §13 such that

$$\operatorname{supp} a^{2m,2l}_\partial(0) \cap \mathrm{WF}_{\mathrm{qsc}}\psi(0) = \emptyset, \tag{14.3}$$

and

$$a_\partial^{2m,2l}(T) \neq 0 \text{ at } \exp(TX)[p]. \tag{14.4}$$

Let $A_\partial^{2m,2l} = \operatorname{Op}((a_\partial^{2m,2l})^{\frac{1}{2}}) \operatorname{Op}((a_\partial^{2m,2l})^{\frac{1}{2}})^*$. Then A_∂ is a non-negative self-adjoint element of $\Psi_{\mathrm{qsc}}^{2m,2l}(M)$ with $\mathrm{WF}'_{\mathrm{qsc}} A_\partial = \operatorname{ell} A_\partial = \operatorname{ess\,supp} a_\partial$.

We know by the symbol calculus of Proposition 6.7 that

$$-\partial_t A - i[\mathcal{H}, A_\partial^{2m,2l}] = (C_\partial^{m+\frac{1}{2},l+\frac{1}{2}})^*(C_\partial^{m+\frac{1}{2},l+\frac{1}{2}}) - E$$

where $C_\partial^{m+\frac{1}{2},l+\frac{1}{2}} = \operatorname{Op}(c_\partial^{m+\frac{1}{2},l+\frac{1}{2}}) \in \Psi_{\mathrm{qsc}}^{m+\frac{1}{2},l+\frac{1}{2}}(M)$ and $E \in \Psi_{\mathrm{qsc}}^{2m,2l+2}(M)$. Thus by Lemma 10.1,

$$\begin{aligned} &\left\langle A_\partial^{2m,2l}\psi_n(s), \psi_n(s)\right\rangle + \int_0^s \left\| C_\partial^{m+\frac{1}{2},l+\frac{1}{2}}\psi_n(t)\right\|^2 dt \\ &\qquad = \left\langle A_\partial^{2m,2l}\psi_n(0), \psi_n(0)\right\rangle + \int_0^s \langle E\psi_n(t), \psi_n(t)\rangle dt, \end{aligned} \tag{14.5}$$

where $\|\cdot\|$ is L^2 norm on M. Thus,

$$\begin{aligned} &\int_0^s \left\| C_\partial^{m+\frac{1}{2},l+\frac{1}{2}}\psi_n(t)\right\|^2 dt \\ &\leqslant -\left\langle A_\partial^{2m,2l}\psi_n(s), \psi_n(s)\right\rangle + \left\langle A_\partial^{2m,2l}\psi_n(0), \psi_n(0)\right\rangle + \int_0^s |\langle E\psi_n(t), \psi_n(t)\rangle| dt \ \forall s \in [0,T]. \end{aligned} \tag{14.6}$$

Now let $V_{m+\frac{1}{2}}$ be the Hilbert space of distributions with norm

$$\left(\int_0^T \|u(t)\|_{m,l}^2 + \left\| C_\partial^{m+\frac{1}{2},l+\frac{1}{2}} u(t)\right\|^2 dt\right)^{\frac{1}{2}}.$$

Equations (14.6) and (14.2) imply that

$$\|\psi_n\|_{V_{m+\frac{1}{2}}} \leqslant c\|\psi_n(0)\|_{m_0,l_0}, \tag{14.7}$$

As $n \to \infty$, the right-hand side goes to $c\|\psi(0)\|_{m_0,l_0}$, so the sequence $\{\psi_n\}$ is bounded in $V_{m+\frac{1}{2}}$. We extract a weakly-convergent subsequence ψ_{n_i}. Since

$$\psi_{n_i} \to \psi \text{ in } L^\infty([0,T]; H_{\mathrm{qsc}}^{m,l}(M)),$$

$\psi \in V_{m+\frac{1}{2}}$ and

$$\|\psi\|_{V_{m+\frac{1}{2}}} \leqslant c\|\psi(0)\|_{m_0,l_0}$$

with the constant c independent of the choice of $\psi(0) \in H_{\mathrm{qsc}}^{m_0,l_0}(M)$.

Let $a_\partial^{2m+1,2l}$ be constructed as in §13 with $\operatorname{supp} a_\partial^{2m+1,2l} \subset (\operatorname{supp} a_\partial^{2m,2l})^\circ$ but still satisfying (14.3) and (14.4). Again applying Lemma 10.1 gives

$$\left\langle A_\partial^{2m+1,2l}\psi_n(s), \psi_n(s)\right\rangle + \int_0^s \left\| C_\partial^{m+1,l+\frac{1}{2}}\psi_n(t)\right\|^2 dt = \left\langle A_\partial^{2m+1,2l}\psi_n(0), \psi_n(0)\right\rangle + \int_0^s \langle E\psi_n(t), \psi_n(t)\rangle dt, \tag{14.8}$$

where now $E \in \Psi_{\mathrm{qsc}}^{2m+1,2l+2}(M)$ is a different operator from that in (14.5), and $\mathrm{WF}'_{\mathrm{qsc}} E \subset \mathrm{WF}'_{\mathrm{qsc}} A_\partial^{2m+1,2l}$.

We can control the E term in (14.8) by using our estimate (14.7): by Proposition 6.14, there exists $Q \in \Psi_{\mathrm{qsc}}^{0,0}(M)$ such that

$$E = (C_\partial^{m+\frac{1}{2},l+\frac{1}{2}})^* Q (C_\partial^{m+\frac{1}{2},l+\frac{1}{2}}) + R$$

with $R \in \Psi_{\mathrm{qsc}}^{-\infty,\infty}(M)$. Thus there exists a constant c (we will keep recycling the letter c to denote uninteresting constants) such that

$$\sup_{t\in[0,T]} |\langle Eu, u\rangle| \leqslant c\|u\|_{V_{m+\frac{1}{2}}}^2, \quad \forall u \in \dot{\mathcal{C}}^\infty(M). \tag{14.9}$$

Applying (14.9) to ψ_n and using (14.7) shows that there is a constant c such that

$$\int_0^s |\langle E\psi_n, \psi_n\rangle| dt \leqslant c\|\psi_n(0)\|_{m_0,l_0}^2, \quad \forall s \in [0,T]. \tag{14.10}$$

This constant is independent of $\psi_n(0) \in \dot{\mathcal{C}}^\infty(M)$. In particular, (14.10) holds for all n.

Using (14.10), we rewrite our basic estimate (14.8) as

$$\left\langle A_\partial^{2m+1,2l}\psi_n(s), \psi_n(s)\right\rangle + \int_0^s \left\| C_\partial^{m+1,l+\frac{1}{2}}\psi_n(t)\right\|^2 dt \leqslant \left\langle A_\partial^{2m+1,2l}\psi_n(0), \psi_n(0)\right\rangle + c\|\psi_n(0)\|_{m_0,l_0}^2 \quad \forall s \in [0,T]. \tag{14.11}$$

Now let V_{m+1} be the Banach space with norm

$$\left(\int_0^T \|u(t)\|_{m,l}^2 + \left\| C_\partial^{m+1,l+\frac{1}{2}} u(t)\right\|^2 dt\right)^{\frac{1}{2}} + \sup_{0\leqslant s\leqslant T} \left\langle A_\partial^{2m+1,2l} u(s), u(s)\right\rangle^{\frac{1}{2}}$$

Equation (14.11) yields

$$\|\psi\|_{V_{m+1}} \leqslant c\left(\left\langle A_\partial^{2m+1,2l}\psi(0), \psi(0)\right\rangle^{\frac{1}{2}} + \|\psi(0)\|_{m_0,l_0}\right). \tag{14.12}$$

This estimate allows us to keep increasing m: we can now plug $A_\partial^{2m+2,2l}$ (again with shrunken operator wavefront set) into Lemma 10.1 and use (14.12) to control the remainder term, and we get

$$\left\langle A_\partial^{2m+2,2l}\psi_n(s),\psi_n(s)\right\rangle+\int_0^s\left\|C_\partial^{m+\frac{3}{2},l+\frac{1}{2}}\psi_n(t)\right\|^2dt$$
$$\leqslant c\left(\left\langle A_\partial^{2m+2,2l}\psi_n(0),\psi_n(0)\right\rangle+\left\langle A_\partial^{2m+1,2l}\psi_n(0),\psi_n(0)\right\rangle+\|\psi_n(0)\|^2_{m_0,l_0}\right),\ \forall s\in[0,T],$$

i.e.

$$\|\psi\|_{V_{m+\frac{3}{2}}}\leqslant c\left(\left\langle A_\partial^{2m+2,2l}\psi(0),\psi(0)\right\rangle^{\frac{1}{2}}+\left\langle A_\partial^{2m+2,2l}\psi(0),\psi(0)\right\rangle^{\frac{1}{2}}+\|\psi(0)\|_{m_0,l_0}\right),$$

and so on. In general,

(14.13)
$$\|\psi\|_{V_{m+\frac{k+1}{2}}}\leqslant c\left(\left\langle A_\partial^{2m+k,2l}\psi(0),\psi(0)\right\rangle^{\frac{1}{2}}+\cdots+\left\langle A_\partial^{2m,2l}\psi(0),\psi(0)\right\rangle^{\frac{1}{2}}+\|\psi(0)\|_{m_0,l_0}\right)$$

where the norm on the Banach space $V_{m+\frac{k+1}{2}}$ is

$$\left(\int_0^T\|u(t)\|^2_{m,l}+\left\|C_\partial^{m+\frac{k+1}{2},l+\frac{1}{2}}u(t)\right\|^2dt\right)^{\frac{1}{2}}+\sup_{0\leqslant s\leqslant T}\left\langle A_\partial^{2m+k,2l}u(s),u(s)\right\rangle^{\frac{1}{2}}$$

The finiteness of $\|\psi\|_{V_{m+\frac{k+1}{2}}}$ gives the desired regularity result for ψ: Let

$$G_k=\mathrm{Op}((a_\partial^{2m+k,2l})^{\frac{1}{2}}),$$

so that $A_\partial^{2m+k,2l}=G_k^*G_k$. Then (14.13) shows that $\|G_k\psi(T)\|^2$ is finite, so since $\exp(TX)[p]\in\operatorname{ell}G_k(T)$, $\exp(TX)[p]\notin\mathrm{WF}_{\mathrm{qsc}}^{m+\frac{k}{2},l+\frac{1}{2}}\psi(T)$ for any k, i.e. $\exp(TX)[p]\notin\mathrm{WF}_{\mathrm{qsc}}\psi(T)$, as desired.

The converse regularity statement follows by time-reversal. □

Proof of Theorem 12.2, part 1. The proof of this result comes in two parts: first, we use the symbol a_+ to prove regularity in a neighborhood of a point $q\in\mathcal{N}_+^c$ given regularity at a point in $\mathcal{N}_+$. Then we use the symbol $a_\circ$ to prove regularity at a point $p\in{}^{\mathrm{qsc}}S^*M\backslash\mathcal{N}_-^c$ such that $N_{-\infty}(p)=q$.

Suppose $q\in\mathcal{N}_+^c$ and $\exp(-TX)[q]\notin\mathrm{WF}_{\mathrm{qsc}}\psi(0)$. Then we can construct $a_+^{2m,2l}$ as described in §13 so that $\mathrm{WF}_{\mathrm{qsc}}\psi(0)\cap\operatorname{supp}a_+(0)=\emptyset$, and $a_+(T)\neq 0$ at q. For the duration of this proof, we are assuming that $l<0$.

Now let

$$A_+^{2m,2l}=\mathrm{Op}((a_+^{2m,2l})^{\frac{1}{2}})^*\,\mathrm{Op}((a_+^{2m,2l})^{\frac{1}{2}})\in\Psi_{\mathrm{qsc}}^{m,l}(M).$$

Then

$$i[\mathcal{H},A_+^{2m,2l}]=(C_+^{m+\frac{1}{2},l+\frac{1}{2}})^*(C_+^{m+\frac{1}{2},l+\frac{1}{2}})+\sum D_i^*D_i-E$$

where $E \in \Psi^{2m,2l+2}_{\mathrm{qsc}}(M)$, $\sum_i D_i^* D_i$ is a finite sum of elements of $\Psi^{2m+1,2l+1}_{\mathrm{qsc}}(M)$, and $\mathrm{WF}'_{\mathrm{qsc}} C_+ \subset \mathrm{WF}'_{\mathrm{qsc}} A_+$.

Lemma 10.1 yields

$$(14.14)\quad \left\langle A_+^{2m,2l}\psi_n(s),\psi_n(s)\right\rangle + \int_0^s \left\| C_+^{m+\frac12,l+\frac12}\psi_n(t)\right\|^2 dt + \sum_i \int_0^s \|D_i\psi_n(t)\|^2 dt = \left\langle A_+^{2m,2l}\psi_n(0),\psi_n(0)\right\rangle + \int_0^s \langle E\psi_n(t),\psi_n(t)\rangle dt,$$

hence

$$(14.15)\quad \int_0^s \left\| C_+^{m+\frac12,l+\frac12}\psi_n(t)\right\|^2 dt \leqslant -\left\langle A_+^{2m,2l}\psi_n(s),\psi_n(s)\right\rangle + \left\langle A_+^{2m,2l}\psi_n(0),\psi_n(0)\right\rangle + \int_0^s |\langle E\psi_n(t),\psi_n(t)\rangle| dt,\ s\in[0,T].$$

Set

$$\|u\|_{V_{m+\frac12}} = \left(\int_0^T \|u(t)\|^2_{m,l} + \left\| C_+^{m+\frac12,l+\frac12}u(t)\right\|^2\right)^{\frac12}.$$

Then (14.15) and (14.2) imply that

$$(14.16)\qquad \|\psi_n\|_{V_{m+\frac12}} \leqslant c\|\psi_n(0)\|_{m_0,l_0}.$$

Hence $\psi \in V_{m+\frac12}$ and $\|\psi\|_{V_{m+\frac12}} \leqslant c\|\psi(0)\|_{m_0,l_0}$.

Now construct $a_+^{2m+1,2l}$ as in §13 with $\operatorname{supp} a_+^{2m+1,2l} \subset (\operatorname{supp} a_+^{2m,2l})^\circ$. Again applying Lemma 10.1 gives

$$\left\langle A_+^{2m+1,2l}\psi_n(s),\psi_n(s)\right\rangle + \int_0^s \left\| C_+^{m+1,l+\frac12}\psi_n(t)\right\|^2 dt + \sum_i \int_0^s \|D_i\psi_n(t)\|^2 dt = \left\langle A_+^{2m+1,2l}\psi_n(0),\psi_n(0)\right\rangle + \int_0^s \langle E\psi_n(t),\psi_n(t)\rangle dt.$$

Here the D_i's and E are not the same as those in (14.14): $D_i^* D_i$ now lies in $\Psi^{2m+2,2l+1}_{\mathrm{qsc}}(M)$ and $E \in \Psi^{2m+1,2l+2}_{\mathrm{qsc}}(M)$. We can control the E term:

$$\int_0^T |\langle E\psi_n(t),\psi_n(t)\rangle| dt \leqslant c\|\psi_n(0)\|^2_{m_0,l_0}$$

by (14.16) and Proposition 6.14. Thus,

$$(14.17)\quad \left\langle A_+^{2m+1,2l}\psi_n(s),\psi_n(s)\right\rangle + \int_0^s \left\| C_+^{m+1,l+\frac12}\psi_n(t)\right\|^2 dt \leqslant \left\langle A_+^{2m+1,2l}\psi_n(0),\psi_n(0)\right\rangle + c\|\psi_n(0)\|^2_{m_0,l_0}$$

Thus if

$$\|u\|_{V_{m+1}} = \left(\int_0^T \|u(t)\|_{m,l}^2 + \left\|C_+^{m+1,l+\frac{1}{2}} u(t)\right\|^2 dt\right)^{\frac{1}{2}} + \sup_{0\leqslant s\leqslant T} \left\langle A_+^{2m+1,2l} u(T), u(T)\right\rangle^{\frac{1}{2}},$$

(14.17) yields

$$\|\psi\|_{V_{m+1}} \leqslant c\left(\left\langle A_+^{2m+1,2l}\psi(0), \psi(0)\right\rangle^{\frac{1}{2}} + \|\psi(0)\|_{m_0,l_0}\right). \tag{14.18}$$

Now iterate:

$$\|\psi\|_{V_{m+\frac{k+1}{2}}} \leqslant c\left(\left\langle A_+^{2m+k,2l}\psi(0), \psi(0)\right\rangle^{\frac{1}{2}} + \cdots + \left\langle A_+^{2m,2l}\psi(0), \psi(0)\right\rangle^{\frac{1}{2}} + \|\psi(0)\|_{m_0,l_0}\right)$$

where the norm on $V_{m+\frac{k+1}{2}}$ is

$$\left(\int_0^T \|\psi(t)\|_{m,l}^2 + \left\|C_+^{m+\frac{k+1}{2},l+\frac{1}{2}}\psi(t)\right\|^2 dt\right)^{\frac{1}{2}} + \sup_{0\leqslant s\leqslant T}\left\langle A_+^{2m+k,2l}\psi(s), \psi(s)\right\rangle^{\frac{1}{2}}.$$

Since by construction, $a_+^{2m+k,2l}(T) \neq 0$ at q for every k, we have $q \notin \mathrm{WF}_{\mathrm{qsc}}\psi(t)$. In fact, since $\operatorname{supp} a_+ \neq 0$ at q for some interval in s, we have $q \notin \mathrm{WF}_{\mathrm{qsc}}^{[T-\delta,T]}\psi$ for some $\delta > 0$. Since $\exp(-TX)[q] \notin \mathrm{WF}_{\mathrm{qsc}}\psi(0)$ is an open condition on T,

$$q \notin \mathrm{WF}_{\mathrm{qsc}}^{[T-\delta,T+\delta]}\psi$$

for some $\delta > 0$. This concludes the proof of regularity at $q \in \mathcal{N}_+^c$.

To finish off the proof, we now use $a_\circ$ to get regularity at time T at *all* points $p \in {}^{\mathrm{qsc}}S^*M$ with $N_{-\infty}(p) = q$. For convenience, we shift t so that $T = \delta/2$; hence the result just proven reads $q \notin \mathrm{WF}_{\mathrm{qsc}}^{[-\delta/2,3\delta/2]}\psi$. Given $p \in N_{-\infty}^{-1}(q)$, construct $a_\circ^{2m,2l}$ as in §13, with epsilons chosen small enough that the non-positive error terms in (13.6) are supported in the complement of $\mathrm{WF}_{\mathrm{qsc}}^{[-\delta/2,3\delta/2]}\psi$ and so that $\operatorname{supp} a_\circ \neq 0$ at p for $t > \delta/4$. Let $A_\circ^{m,l} = \mathrm{Op}((a_\circ^{m,l})^{\frac{1}{2}})^* \,\mathrm{Op}((a_\circ^{m,l})^{\frac{1}{2}})$. Then Lemma 10.1 yields

$$\begin{aligned}\left\langle A_\circ^{2m,2l}\psi_n(s), \psi_n(s)\right\rangle + \int_0^s \left\|C_\circ^{m+\frac{1}{2},l+\frac{1}{2}}\psi_n(t)\right\|^2 dt + \sum_i \int_0^s \|E_i\psi_n(t)\|^2 dt \\ = \left\langle A_\circ^{2m,2l}\psi_n(0), \psi_n(0)\right\rangle + \int_0^s \left\langle (E + F^{2m+1,2l+1})\psi_n(t), \psi_n(t)\right\rangle dt\end{aligned} \tag{14.19}$$

where $C_\circ = \mathrm{Op}(c_\circ)$, $E \in \Psi_{\mathrm{qsc}}^{2m,2l+2}(M)$, and $\mathrm{WF}'_{\mathrm{qsc}}F \cap \mathrm{WF}_{\mathrm{qsc}}^{[0,\delta]}\psi = \emptyset$. Since A vanishes at $t = 0$, the term $\langle A_\circ^{2m,2l}\psi_n(0), \psi_n(0)\rangle$ is identically zero. The E term is controlled by the assumed regularity of ψ, so

$$\int_0^\delta \|\psi(t)\|^2_{m,l} + \left\| C_\circ^{m+\frac{1}{2},l+\frac{1}{2}} \psi(t) \right\|^2 dt$$
$$< c \left(\|\psi(0)\|^2_{m_0,l_0} + \int_0^\delta \left| \left\langle F^{2m+1,2l+1} \psi(t), \psi(t) \right\rangle \right| dt \right).$$

Now construct $a_\circ^{2m+1,2l}$, $a_\circ^{2m+2,2l}$, etc. and iterate the argument to obtain

$$\int_0^\delta \|\psi(t)\|^2_{m,l} + \left\| C_\circ^{m+\frac{k+1}{2},l+\frac{1}{2}} \psi(t) \right\|^2 dt + \sup_{0\leqslant s\leqslant \delta} \left\langle A_\circ^{2m+k,2l} \psi(s), \psi(s) \right\rangle$$
$$< c \left(\|\psi(0)\|^2_{m_0,l_0} + \int_0^\delta \left| \left\langle F^{2m+1,2l+1} \psi(t), \psi(t) \right\rangle \right| + \cdots + \left| \left\langle F^{2m+k+1,2l+1} \psi(t), \psi(t) \right\rangle \right| dt \right)$$

for all $k \in \mathbb{Z}_+$. All terms on the right are finite for all k. Thus since $a_\circ \neq 0$ at p for $t > \delta/4$, we have $p \notin \mathrm{WF}_{\mathrm{qsc}}^{[\delta/4,\delta]}\psi$, hence in our original time coordinate,

$$p \notin \mathrm{WF}_{\mathrm{qsc}}^{[T-\delta/4,T+\delta/2]}\psi,$$

as desired. □

Proof of Theorem 12.3, part 1. It will suffice to prove that $q \notin \mathrm{WF}_{\mathrm{qsc}}\psi(t)$ for t sufficiently small: since $\mathrm{WF}_{\mathrm{qsc}}$ is closed, some neighborhood of q in ${}^{\mathrm{qsc}}\overline{T}^*_{\partial M}M$ is then absent from $\mathrm{WF}_{\mathrm{qsc}}\psi(t)$ as well, and in particular, $\exp(\epsilon X)[q] \notin \mathrm{WF}_{\mathrm{qsc}}\psi(\epsilon)$ for some $\epsilon > 0$; Theorem 12.1 will suffice to complete the proof.

We can take $l > 0$ for the duration of this proof.

We can construct $a_-^{2m,2l}$ as in §13 such that the non-positive terms in $(-\partial_t - X)a_-$ are supported in the complement of $\mathrm{WF}_{\mathrm{qsc}}^{[-\delta,\delta]}\psi$. Now let

$$A_-^{2m,2l} = \mathrm{Op}((a_-^{2m,2l})^{\frac{1}{2}})^* \, \mathrm{Op}((a_-^{2m,2l})^{\frac{1}{2}})$$

and $C_- = \mathrm{Op}(c_-)$. The positive commutator argument works just like the preceding ones. □

Proof of Theorem 12.4. No further positive commutator arguments are required: Theorem 12.4 is a corollary of Theorems 12.1, 12.2, and 12.3.

We have assumed that the corner point $\exp(-\lambda_0^{-1}X)[p]$ is not backward-trapped. Hence, by Theorem 11.6, there is a neighborhood O of this point in $\mathcal{N}_-^c$ such that $O \cap \mathcal{T}_- = \emptyset$. By Theorem 11.6 and since $\mathrm{WF}_{\mathrm{qsc}}$ is closed, we can further assume that

$$\exp(-(T-\lambda_0^{-1})X)\,[\mathsf{Scat}(O)] \cap \mathrm{WF}_{\mathrm{qsc}}\psi(0) = \emptyset.$$

Now applying the first part of Theorem 12.2 tells us that

$$N_{-\infty}^{-1}\,[\mathsf{Scat}(O)] \tag{14.20}$$

is disjoint from $\mathrm{WF}_{\mathrm{qsc}}^{[T-\lambda_0^{-1}-\delta, T-\lambda_0^{-1}+\delta]}\psi$ for some $\delta > 0$. By definition of Scat, the set (14.20) contains $N_{+\infty}^{-1}(O)$. Thus we may apply Theorem 12.3 to conclude that $p \notin \mathrm{WF}_{\mathrm{qsc}}\psi(T)$. □

Proof of Theorem 12.5. This proof is essentially a combination of those of Theorems 12.2 and 12.3. First, let p' be any point in $\mathsf{Scat}(q)$. By our wavefront assumption and by Theorems 12.1 and 12.2, we can construct a symbol $\tilde{a}_+^{m,l}$ with $\tilde{a}_+^{m,l} \neq 0$ at p' and $\operatorname{supp} \tilde{a}_+^{m,l} \cap \mathrm{WF}_{\mathrm{qsc}}^{[0,\delta]}\psi = \emptyset$ for some $\delta > 0$ independent of the choice of p' (recall that $\mathsf{Scat}(q)$ is a closed set). Then using the same notational conventions as above, we have

$$
\begin{aligned}
(14.21)\quad & \left\langle \tilde{A}_+^{2m,2l}\psi(s), \psi(s) \right\rangle + \int_0^s \left\| \tilde{C}_+^{m+\frac{1}{2},l+\frac{1}{2}}\psi(t) \right\|^2 dt + \sum_i \int_0^s \|D_i\psi(t)\|^2 dt \\
&= \left\langle \tilde{A}_+^{2m,2l}\psi_n(0), \psi_n(0) \right\rangle + \int_0^s \langle E\psi(t), \psi(t)\rangle dt - \int_0^s \left\langle G^{2m+1,2l+1}\psi(t), \psi(t) \right\rangle dt;
\end{aligned}
$$

since $\mathrm{WF}'_{\mathrm{qsc}}G$ is contained in the complement of $\mathrm{WF}^{[0,\delta]}\psi$, the $\int_0^s \langle G\psi, \psi\rangle dt$ term is finite if $s \leqslant \delta$, and the usual iterative argument gives

$$
\begin{aligned}
&\int_0^\delta \|\psi(s)\|_{m,l}^2 + \left\| \tilde{C}_+^{m+\frac{k+1}{2},l+\frac{1}{2}}\psi(s) \right\|^2 ds + \sup_{0\leqslant s\leqslant \delta} \left\langle \tilde{A}_+^{2m+k,2l}\psi(s), \psi(s) \right\rangle \\
&\quad < c\Bigg(\|\psi(0)\|_{m_0,l_0}^2 + \left\langle \tilde{A}_+^{2m+k,2l}\psi(0), \psi(0) \right\rangle + \cdots + \left\langle \tilde{A}_+^{2m,2l}\psi(0), \psi(0) \right\rangle \\
&\qquad + \int_0^\delta \left| \left\langle G^{2m+1,2l+1}\psi(s), \psi(s) \right\rangle \right| + \cdots + \left| \left\langle G^{2m+k+1,2l+1}\psi(s), \psi(s) \right\rangle \right| ds \Bigg).
\end{aligned}
$$

The $\left\langle \tilde{A}_+\psi(0), \psi(0) \right\rangle$ terms are finite by our wavefront assumption, and the $\langle G\psi, \psi\rangle$ terms are finite since $\operatorname{supp} g \cap \mathrm{WF}_{\mathrm{qsc}}^{[0,\delta]}\psi = \emptyset$. Thus $\operatorname{supp} a_+ \cap \mathrm{WF}_{\mathrm{qsc}}^{[0,\delta]}\psi = \emptyset$, hence a neighborhood of $\mathsf{Scat}(q)$ in ${}^{\mathrm{qsc}}S^*M$ is absent from $\mathrm{WF}_{\mathrm{qsc}}^{[0,\delta]}\psi$.

Thus given any $p' \in N_{+\infty}^{-1}(q)$, since $N_{-\infty}(p') \in \mathsf{Scat}(q)$ we can construct a symbol $\tilde{a}_\circ$ nonzero at p' such that the non-positive terms in $(-\partial_t - X)\tilde{a}_\circ$ are contained in the complement of $\mathrm{WF}_{\mathrm{qsc}}^{[0,\delta]}\psi$ and such that $\operatorname{supp} \tilde{a}_\circ$ is contained in a small enough neighborhood of $N_{+\infty}^{-1}(q)$ that it does not meet $\mathrm{WF}_{\mathrm{qsc}}\psi(0)$. Then the same argument as used for $\tilde{a}_+$ shows that $\operatorname{supp} \tilde{c}_\circ \cap \mathrm{WF}_{\mathrm{qsc}}^{[0,\delta]} = \emptyset$. Hence we have shown that

$$
N_{+\infty}^{-1}(q) \cap \mathrm{WF}_{\mathrm{qsc}}^{[0,\delta]}\psi = \emptyset.
$$

We can now construct the symbol $\tilde{a}_-$ supported in a neighborhood of q such that $\operatorname{supp} g \cap \mathrm{WF}_{\mathrm{qsc}}^{[0,\delta]}\psi = \emptyset$, and use the now-usual argument to obtain $q \notin \mathrm{WF}_{\mathrm{qsc}}^{[0,\delta]}\psi$. Since $\mathrm{WF}_{\mathrm{qsc}}$ is closed, Theorem 12.1 takes care of the rest. □

References

[1] Boutet de Monvel, L., Propagation des singularités des solutions d'équations analogues à l'équation de Schrödinger, *Fourier integral operators and partial differential operators*, Springer Lecture Notes in Mathematics, *459* (1975), 1-14.

[2] Cordes, H. O., A global parametrix for pseudodifferential operators over $\mathbb{R}^n$ with applications, preprint No. 90, SFB 72, Bonn, 1976.

[3] Craig, W., *Les moments microlocaux et la regularité des solutions de l'equation de Schrödinger,* Ecole Polytechnique séminaire 'Equations aux Dérivées Partielles,' Exposée XX.

[4] Craig, W., Kappeler, T., and Strauss, W., Microlocal dispersive smoothing for the Schrödinger equation, *Comm. Pure Appl. Math.*, **48** (1995), 769–860.

[5] Doi, S.-I., Smoothing effects of Schrödinger evolutions groups on Riemannian manifolds, *Duke Math. J.*, **82** (1996), 679–706.

[6] Epstein, C. L., Melrose, R. B., and Mendoza, G. A., Resolvent of the Laplacian on strictly pseudoconvex domains, *Acta Math.*, **167** (1991), 1–106.

[7] Fujiwara, D., Remarks on the convergence of the Feynman path integrals, *Duke Math. J.*, **47** (1980), 559–600.

[8] Hörmander, L., On the existence and the regularity of solutions of linear pseudo-differential equations, *L'Enseignement Math.*, **17** (1971), 99–163.

[9] Hörmander, L. Fourier integral operators I, *Acta Math.*, **127** (1971), 79–183.

[10] Hörmander, L. *The analysis of linear partial operators III*, Springer Verlag, Berlin Heidelberg New York Tokyo, 1985.

[11] Kapitanski, L., Rodnianski, I., and Yajima K., On the fundamental solution of a perturbed harmonic oscillator, *Topol. Methods Nonlinear Anal.*, **9** (1997), 77–106.

[12] Kapitanski, L. and Safarov, Y., Dispersive smoothing for Schrödinger equations, *Math. Res. Lett.*, **3** (1996), 77–91.

[13] Kosinski, A. A., *Differential manifolds,* Academic Press, San Diego, 1993.

[14] Lascar, R., Propagation des singularités des solutions d'équations pseudo-differentielles quasi-homogenes, *Ann. Inst. Fourier*, **27** (1977), 79-123.

[15] Melrose, R. B., Spectral and scattering theory for the Laplacian on asymptotically Euclidean spaces, *Spectral and scattering theory* (M. Ikawa, ed.), Marcel Dekker, 1994.

[16] Melrose, R. B., *Geometric scattering theory*, Cambridge University Press, Cambridge New York Melbourne, 1995.

[17] Melrose, R. B., *Differential analysis on manifolds with corners,* in preparation.

[18] Melrose, R. B. and Zworski, M., Scattering metrics and geodesic flow at infinity, *Inv. Math.*, **124** (1996), 389–436.

[19] Parenti, C., Operatori pseudodifferentiali in $\mathbb{R}^n$ e applicazioni, *Ann. Math. Pura Appl.* **93** (1972), 359–389.

[20] Schrohe, E., Spaces of weighted symbols and weighted Sobolev spaces on manifolds, *Pseudodifferential operators, Proceedings, Oberwolfach 1986*, Lecture Notes in Mathematics **1256**, Springer Verlag, Berlin Heidelberg New York Tokyo, 1987.

[21] Schrohe, E., Complex powers on noncompact manifolds and manifolds with singularities, *Math. Ann.* **281** (1988), 393–409.

[22] Sell, G., Smooth linearization near a fixed point, *Amer. J. Math.*, **107** (1985), 1035–1091.

[23] Shananin, N. A., On singularities of solutions of the Schrödinger equation for a free particle, *Matematicheskie Zametki* **55** (1994), 116–123, *Math. Notes* **55** (1994), 626–631.

[24] Shubin, M. A., Pseudodifferential operators in $\mathbb{R}^n$, *Dokl. Akad. Nauk SSSR*, **196** No. 2 (1971), 316–319, *Soviet Math. Dokl.* **12**, No.1 (1971), 147–151.

[25] Sigal, I. M. and Soffer, A., Long-range many-body scattering. Asymptotic clustering for Coulomb-type potentials, *Invent. Math.*, **99** (1990), 115–143.

[26] Sternberg, S., Local contractions and a theorem of Poincaré, *Amer. J. Math.*, **79** (1957), 809–824.
[27] Treves, F., Parametrices for a class of Schrödinger equations, *Comm. Pure Appl. Math.*, **48** (1995), 13–78.
[28] Weinstein, A., A symbol class for some Schrödinger equations on $\mathbb{R}^n$, *Amer. J. Math.*, **107** (1985), 1–21.
[29] Yajima, K., Smoothness and non-smoothness of the fundamental solution of time-dependent Schrödinger equations, *Comm. Math. Phys.* **181** (1996), 605–629.
[30] Zelditch, S., Reconstruction of singularities for solutions of Schrödinger equations, *Comm. Math. Phys.* **90** (1983), 1–26.

E-mail address: `jwunsch@math.harvard.edu`

Department of Mathematics, Harvard University, 1 Oxford St. Rm. 325, Cambridge MA 02138