PROPAGATION OF SINGULARITIES IN THREE-BODY SCATTERING

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Abstract. In this paper we consider a compact manifold with boundary X equipped with a scattering metric g and with a collection C_i of disjoint closed embedded submanifolds of ∂X. Thus, g is a Riemannian metric in $\mathrm{int}(X)$ of the form $g = x^{-4}\,dx^2 + x^{-2}h$ near ∂X for some choice of a boundary defining function x, h being a smooth symmetric 2-cotensor on X which is non-degenerate when restricted to ∂X. We also let Δ be the (positive) Laplacian of g, suppose that $V \in \mathcal{C}^\infty([X;\cup_i C_i])$ where $[X;\cup_i C_i]$ is X blown up along the C_i, assume that V vanishes at the lift of ∂X, and consider the operator $H = \Delta + V$. Three-body scattering with smooth potentials which have an asymptotic expansion at infinity (possibly Coulomb-type) provide the standard example of this setup. We analyze the propagation of singularities of generalized eigenfunctions of H, showing that this is essentially a hyperbolic problem which has much in common with the Dirichlet and transmission problems for the wave operator, though additional features arise due to the presence of bound states of the 'two-body operators'. We also show that the wave front relation of the free-to-free part of the scattering matrix is given by the broken geodesic flow at distance π.

Contents

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1. Introduction

Let X be a compact manifold with boundary. In [22] Melrose has defined the algebra $\mathrm{Diff}_{\mathrm{sc}}(X)$ of scattering differential operators on X. In fact, let $x \in \mathcal{C}^\infty(X)$ be a boundary defining function of X, so $x \geq 0$, $dx \neq 0$ on ∂X, and $\partial X = \{x = 0\}$. The Lie algebra of b-vector fields on X, $\mathcal{V}_{\mathrm{b}}(X)$, is the set of all smooth vector fields on X which are tangent to ∂X. The Lie algebra of scattering vector fields on X, $\mathcal{V}_{\mathrm{sc}}(X)$, is simply $\mathcal{V}_{\mathrm{sc}}(X) = x\mathcal{V}_{\mathrm{b}}(X)$; this notion is independent of the choice of the boundary defining function x. Much as in the case of $\mathcal{V}_{\mathrm{b}}(X)$, $\mathcal{V}_{\mathrm{sc}}(X)$ is the set of all smooth sections of a vector bundle over X; this bundle is denoted by ${}^{\mathrm{sc}}TX$. Finally, $\mathrm{Diff}_{\mathrm{sc}}(X)$ is just the enveloping algebra of $\mathcal{V}_{\mathrm{sc}}(X)$, i.e. the ring of operators on $\mathcal{C}^\infty(X)$ generated by $\mathcal{C}^\infty(X)$ (considered as multiplication operators) and $\mathcal{V}_{\mathrm{sc}}(X)$. An example of such an operator is the Laplacian Δ associated to a scattering metric g. Thus, g is a Riemannian metric in $\mathrm{int}(X)$ of the form $g = x^{-4}\,dx^2 + x^{-2}h$ near ∂X for some choice of a boundary defining function x, h being a smooth symmetric 2-cotensor on X which is non-degenerate when restricted to ∂X. In particular, g is a metric on ${}^{\mathrm{sc}}TX$.

Let C_i, $i = 1, \ldots, k$, be disjoint closed embedded submanifolds of ∂X. Here the C_i might have different dimensions. Nevertheless, to simplify the notation, we introduce $C = \cup_i C_i$, and say that C is also a closed embedded submanifold of ∂X, although this is strictly speaking only true if the dimensions of the connected components of C are the same. Let mf ('main face') be the lift of ∂X to $[X; C]$, the blow-up of X along C (see the Appendix of [22] for a treatment of blow-ups, and see Figure 1 for a picture). We write ρ_{mf} for a defining function of mf. The 'three-body type' operators we are interested in are perturbations H of Δ of the form $H = \Delta + V$, where $V \in \mathcal{C}^\infty([X; C])$ is real-valued and vanishes at mf. As discussed in the following paragraphs, three-body Hamiltonians, with the center of mass removed, give an example of such operators, and explain our interest in the problem. In the degenerate case when $k = 0$, i.e. $C = \emptyset$, we arrive at the generalized 'two-body type' scattering considered in Melrose's original paper [22]; in this case $V \in x\mathcal{C}^\infty(X)$.

Consider the Euclidian space, $\mathbb{R}^N$, with the standard metric, and its radial compactification to the upper hemisphere $\mathbb{S}^N_+$. Embedding $\mathbb{S}^N_+$ in $\mathbb{R}^{N+1}$ as the unit upper hemisphere this is given by the map $\mathrm{SP} : \mathbb{R}^N \to \mathbb{S}^N_+$

$$\mathrm{SP}(z) = \left(\frac{1}{(1+|z|^2)^{1/2}}, \frac{z}{(1+|z|^2)^{1/2}} \right). \tag{1.1}$$

Let x be a boundary defining function of $\mathbb{S}^N_+$ such that $x = (\mathrm{SP}^{-1})^*|z|^{-1}$ near $\partial\mathbb{S}^N_+$. Then the Euclidian metric pulls back to a scattering metric on $\mathbb{S}^N_+$, with h being the standard metric on $\mathbb{S}^{N-1} = \partial\mathbb{S}^N_+$, and the Euclidian Laplacian becomes an element of $\mathrm{Diff}^2_{\mathrm{sc}}(\mathbb{S}^N_+)$.

Let X_i, $i = 1, \ldots, k$, be linear subspaces of $\mathbb{R}^N$, let X^i be the orthocomplement of X_i, $n_i = \dim X^i$, and let π^i be the orthogonal projection to X^i. By a Euclidian many-body Hamiltonian we mean an operator of the form $H = \Delta + \sum_i (\pi^i)^* V_i$

where $V_i \in \mathcal{C}^\infty(X^i;\mathbb{R})$ satisfy $(\mathrm{SP}_i^{-1})^* V_i \in \rho_i \mathcal{C}^\infty(\mathbb{S}_+^{n_i})$ with ρ_i denoting a boundary defining function of $\mathbb{S}_+^{n_i}$, and SP_i being the radial compactification map $\mathrm{SP}_i : X^i \to \mathbb{S}_+^{n_i}$. The condition on V_i means that it is a one-step polyhomogeneous symbol on X^i of order -1. A Euclidian three-body Hamiltonian (with center of mass removed) is a many-body Hamiltonian with the additional assumption that $X_i \cap X_j = \{0\}$ for $i \neq j$. In the compactified picture, writing $\overline{X_i} = \mathrm{cl}(\mathrm{SP}(X_i)) \subset \mathbb{S}_+^N$, $C_i = \overline{X_i} \cap \mathbb{S}^{N-1}$, the condition $X_i \cap X_j = \{0\}$ for $i \neq j$ becomes $C_i \cap C_j = \emptyset$ for $i \neq j$. With the notation $C = \cup_i C_i$ as in the general case, it is straightforward to check that

$$V = (\mathrm{SP}^{-1})^* \sum_i (\pi^i)^* V_i \in \mathcal{C}^\infty([\mathbb{S}_+^N; C]), \qquad V|_{\mathrm{mf}} = 0 \tag{1.2}$$

(this will be done here in Lemma 2.1), so H is indeed a 'three-body type' operator as described above in the geometric setting. Note also that the C_i are 'subspheres' of $\mathbb{S}^{N-1}$, in particular, they are totally geodesic with respect to the standard metric. A two-body Hamiltonian corresponds to taking $k = 1$, $X_1 = \{0\}$ above, so we have $V \in x\mathcal{C}^\infty(\mathbb{S}_+^N)$, giving rise to the 'two-body type' terminology in the geometric setting. In Figure 1 below we take $N = 2$ and the X_i are lines. Hence, $X = \mathbb{S}_+^2$ is a disk, $\partial X = \mathbb{S}^1$, each C_i consists of two points. The lift of C_i to $[X;C]$ is denoted by ff_i in the figure.

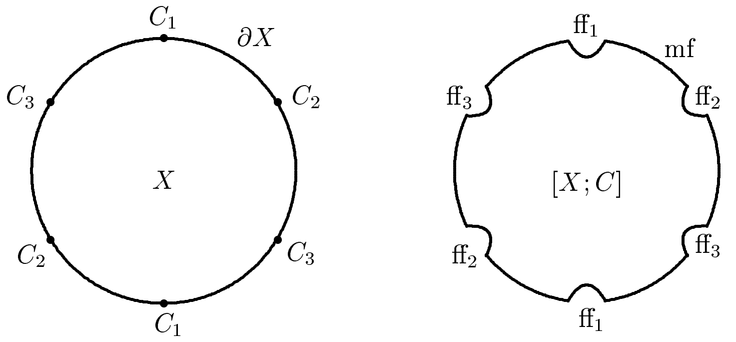

FIGURE 1. The original space X and its resolution $[X;C]$.

Now we return to the general setting. First note that $H = \Delta + V$ is self-adjoint on $L^2_{\mathrm{sc}}(X)$, the L^2 space defined by integration with respect to the Riemannian density dg, since Δ and V are such and V is bounded. Hence, its resolvent $R(\lambda) = (H-\lambda)^{-1}$ is a bounded linear operator on $L^2_{\mathrm{sc}}(X)$ for $\lambda \in \mathbb{C} \setminus \mathbb{R}$. In this paper we analyze the boundary value of the resolvent at the real axis, i.e. $R(\lambda \pm i0)$. We show that $\mathrm{spec}_p(H) \cap (0,\infty) = \emptyset$ and

$$R(\lambda \pm i0) \in \mathcal{B}(x^{1/2+\epsilon} L^2_{\mathrm{sc}}(X), x^{-1/2-\epsilon} L^2_{\mathrm{sc}}(X)) \tag{1.3}$$

for all $\epsilon > 0$. This is completely analogous to the classical result of Mourre in Euclidian three-body scattering ([27, 28], see also the paper [29] of Perry, Sigal and Simon in which they extend Mourre's results to many-body systems), together with the absence of positive eigenvalues which was shown by Froese and Herbst [7] in the Euclidian case.

We also show that for $f \in \dot{\mathcal{C}}^\infty(X)$, $R(\lambda \pm i0) f$ has a complete asymptotic expansion away from C which is similar to the corresponding expansion for Euclidian two-body Hamiltonians. Here $\dot{\mathcal{C}}^\infty(X)$ is the subspace of $\mathcal{C}^\infty(X)$ consisting of functions which vanish at ∂X together with all of their derivatives. For simplicity here we only state the asymptotic expansion if $V \in \rho_{\mathrm{mf}}^2 \mathcal{C}^\infty([X;C])$ (i.e. short-range); the general case is described in Theorem 18.6. It is convenient to replace the spectral parameter λ by λ^2. Then, for $\lambda > 0$, $f \in \dot{\mathcal{C}}^\infty(X)$, the expansion can be described by

$$v_\pm = e^{\pm i\lambda/x} x^{-(N-1)/2} R(\lambda^2 \mp i0) f \in \mathcal{C}^\infty(X \setminus C). \tag{1.4}$$

The top term of such an expansion for Euclidian three-body scattering was described by Isozaki in [18], assuming that the potentials were short range, by Herbst and Skibsted in [14] in the long-range many-body Euclidian case, and the full expansion was proved by the author in [35]. Moreover, we show that given any 'initial data' $a_0 \in \mathcal{C}_c^\infty(\partial X \setminus C)$ we can find $f \in \dot{\mathcal{C}}^\infty(X)$ such that with v_- as above we have $v_- \in \mathcal{C}^\infty(X)$ and $a_0 = v_-|_{\partial X}$. Then

$$u = R(\lambda^2 + i0) f - R(\lambda^2 - i0) f \in \mathcal{C}^{-\infty}(X) \tag{1.5}$$

satisfies $(H - \lambda)u = 0$, and has the form

$$u = e^{i\lambda/x} x^{(N-1)/2} v_- - e^{-i\lambda/x} x^{(N-1)/2} v_+. \tag{1.6}$$

For $\lambda > 0$ the Poisson operator corresponding to 'free initial data' is the map $P(\lambda) : \mathcal{C}_c^\infty(\partial X \setminus C) \to \mathcal{C}^{-\infty}(X)$ given by $P(\lambda) a_0 = u$. This definition is justified by the uniqueness statement of Theorem 19.1 which is again an analog of Isozaki's result [19]. The free-to-free part of the scattering matrix, $S(\lambda)$, relates the leading part of the expansions in (1.6) at $\partial X \setminus C$. Thus, $S(\lambda)$ is the map

$$S(\lambda) : \mathcal{C}_c^\infty(\partial X \setminus C) \to \mathcal{C}^\infty(\partial X \setminus C) \tag{1.7}$$

given by

$$S(\lambda) a_0 = -v_+|_{\partial X \setminus C}, \qquad a_0 \in \mathcal{C}_c^\infty(\partial X \setminus C). \tag{1.8}$$

The equivalence of this definition of the scattering matrix with the customary one involving the wave operators was proved by Hassell [11] for short-range interactions. Here, in Remark 19.12, we sketch a somewhat different proof based on Isozaki's argument in [17].

Our main theorem describes the structure of $S(\lambda)$. We first introduce the broken geodesic flow of $h|_{\partial X}$ on ∂X, broken at C. For simplicity we only define this here if C is totally geodesic; for the general definition see Definition 11.6 and the remarks preceeding it. Let $I \subset \mathbb{R}$ be an interval, and let B be a discrete subset. We denote by $S\partial X$ the sphere bundle of ∂X identified as the unit-length subbundle of $T\partial X$ with respect to $h|_{\partial X}$ (we drop the restriction in the notation from now on). We say that a curve $\gamma : I \to \partial X$ is a broken geodesic of h if two conditions are satisfied. First, for all intervals $J \subset I \setminus B$, $\gamma|_J$ is a geodesic of h, such that for all $t \in J$, $\gamma'(t) \in S\partial X$. Second, if $t \in B$ then $\gamma(t) \in C$ and the limits $\gamma'(t-0)$ and $\gamma'(t+0)$ both exist and differ by a vector in $T_{\gamma(t)}\partial X$ which is orthogonal to $T_{\gamma(t)}C$ (i.e. the usual law of reflection is satisfied; see Figure 2). We say that $p, q \in S\partial X$ are related by the broken geodesic flow at time $-\pi$ if there is a broken geodesic γ defined on $[-\pi, 0]$, such that $\gamma'(0) = p$, $\gamma'(-\pi) = q$. Using the metric h to identify $S\partial X$ and $S^*\partial X$, this defines the broken geodesic flow at time $-\pi$ on $S^*\partial X$. We then have the following result:

Theorem. *For $\lambda > 0$ the wave front relation of the free-to-free part of the scattering matrix, $S(\lambda)$, is given by the broken geodesic flow of $h|_{\partial X}$ on ∂X, broken at C, at time $-\pi$.*

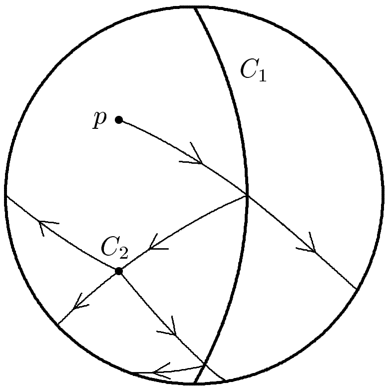

FIGURE 2. Broken geodesics on $\partial X = \mathbb{S}^2$ starting at p.

This theorem was conjectured by Melrose based on his work with Zworski in the generalized 'two-body type' setting [22, 26]. As mentioned above, this just means that we take $C = \emptyset$. The result of Melrose and Zworski was that $S(\lambda)$ is a Fourier integral operator associated to the geodesic flow on ∂X at time $-\pi$, from which our Theorem follows when $C = \emptyset$.

In the case of Euclidian three-body scattering with rapidly decreasing two-body potentials a somewhat stronger result than the Theorem has been proved by the author in [36] by an explicit construction resembling Faddeev's original one [6]; namely the scattering matrix was shown to be a sum of Fourier integral operators associated to the broken geodesic flow. Using different methods, which are closer to those of Melrose and Zworski in [26], Hassell has shown in [12] that the same conclusion holds. In addition, Hassell's construction states explicitly that the kernel of the Poisson operator is a sum of Legendrian distributions associated to conic Legendrian pairs.

We also remark that there are other interesting operators associated to this geometry; one example is Christiansen's analysis of scattering in perturbed stratified media [2].

A major difference between two-body and three-body type scattering is that in the latter case the range of $P(\lambda)$, considered as an operator on $\mathcal{C}^\infty_c(\partial X \setminus C)$, may not be dense in the nullspace of $H - \lambda$ on $\mathcal{C}^{-\infty}(X)$. Apart from those corresponding to 'free initial data', essentially characterized by restriction of their expansion to mf, there are generalized eigenfunctions of $H - \lambda$ corresponding to 'two-body bound states'; in the case of Euclidian three-body scattering these arise from eigenfunctions of $\Delta_{X^i} + V_i$ in $L^2(X^i)$. In the Euclidian setting these are easier to describe than those coming from free initial data; this was done by Isozaki [17, 18] and Skibsted [34] for short-range potentials, and by Bommier [1] for long-range potentials in a more general Euclidian many-body setting. Due to the lack of product structure, this task is much harder in the geometric setting, and we only prove the propagation of singularities of generalized eigenfunctions along bicharacteristics under additional assumptions. These assumptions guarantee that the spectrum of the two-body operators is constant along C, and are satisfied in the Euclidian setting. Even in these cases we do not treat the Poisson operator with initial data in a two-body bound state and the corresponding pieces of the scattering matrix. Hence, we do not consider whether every generalized eigenfunction arises from a combination of 'free' and 'two-body bound' initial data. An L^2 version of this statement is called asymptotic completeness in the Euclidian case; it was proved by Enss [4, 5] for both short-range and long-range three-body scattering. In the many-body setting these were proved by Sigal and Soffer [31, 32], Graf [10], Dereziński [3] and Yafaev [38].

To see why a result such as the above Theorem should hold, consider first the operator $\Delta-\lambda$, and its analysis in Melrose's paper [22]. There is a principal symbol map

$$\sigma_{\mathrm{sc},m}:\mathrm{Diff}^m_{\mathrm{sc}}(X)\to S^m_h({}^{\mathrm{sc}}T^*X), \tag{1.9}$$

$S^m_h({}^{\mathrm{sc}}T^*X)$ denoting the space of homogeneous functions of degree m on ${}^{\mathrm{sc}}T^*X\setminus 0$; this is completely analogous to the principal symbol map on compact manifolds without boundary. We have $\sigma_{\mathrm{sc},2}(\Delta-\lambda)=|\zeta|^2$, $|.|$ denoting the metric function on ${}^{\mathrm{sc}}T^*X$, the dual bundle of ${}^{\mathrm{sc}}TX$. This is independent of λ, and it is elliptic in the usual sense, i.e. it has an inverse in $S^{-2}_h({}^{\mathrm{sc}}T^*X)$. However, $\sigma_{\mathrm{sc},m}$ does not capture the behavior of $\mathrm{Diff}^m_{\mathrm{sc}}(X)$ completely, such as its compactness properties between certain Sobolev spaces. In fact, there is a symbol map, $\hat N_{\mathrm{sc}}$, at ∂X as well, mapping

$$\hat N_{\mathrm{sc}}:\mathrm{Diff}_{\mathrm{sc}}(X)\to\mathcal{C}^\infty({}^{\mathrm{sc}}T^*_{\partial X}X). \tag{1.10}$$

Now, $\hat N_{\mathrm{sc}}(\Delta-\lambda)=|\zeta|^2-\lambda$, i.e. λ is not lower order than Δ in this sense, meaning that it appears in $\hat N_{\mathrm{sc}}(\Delta-\lambda)$. Hence, for $\lambda\geq 0$, $\hat N_{\mathrm{sc}}(\Delta-\lambda)$ is not invertible in $\mathcal{C}^\infty({}^{\mathrm{sc}}T^*_{\partial X}X)$, so $\Delta-\lambda$ is not fully elliptic. *This* gives rise to scattering theory.

It is perhaps useful to remark that if $X=\mathbb{S}^N_+$ is the radial compactification of $\mathbb{R}^N$, $\mathcal{F}$ is the Fourier transform on $\mathbb{R}^N$ (regarded as an operator acting on $\mathcal{C}^{-\infty}(\mathbb{S}^N_+)$) and $P\in\mathrm{Diff}^m_{\mathrm{sc}}(\mathbb{S}^N_+)$ then $\tilde P=\mathcal{F}P\mathcal{F}^{-1}\in\Psi^0(\mathbb{R}^N)$; here $\Psi^0(\mathbb{R}^N)$ is the standard pseudo-differential calculus on $\mathbb{R}^N$. (In fact, $\tilde P\in\Psi^{0,-m}_{\mathrm{sc}}(\mathbb{S}^N_+)$; $\Psi^{\infty,-\infty}_{\mathrm{sc}}(\mathbb{S}^N_+)$ is the microlocalization of $\mathrm{Diff}_{\mathrm{sc}}(\mathbb{S}^N_+)$, see [22].) Moreover, $\hat N_{\mathrm{sc}}(P)$ is closely related to $\sigma_0(\tilde P)$. Namely, with $L:{}^{\mathrm{sc}}T^*_{\mathbb{S}^{N-1}}\mathbb{S}^N_+\to S^*\mathbb{R}^N$ being the Legendre diffeomorphism given in [26, Lemma 5], we have $\sigma_0(\tilde P)=(L^{-1})^*\hat N_{\mathrm{sc}}(P)$. If $P=\Delta-\lambda$, Δ being the standard Euclidian Laplacian, we have $\tilde P=|\zeta|^2-\lambda\in\mathrm{Diff}^0(\mathbb{R}^N)$ (i.e. a multiplication operator). We see directly here that $\tilde P$ is not elliptic (in the usual sense) if $\lambda\geq 0$ since its principal symbol vanishes on the sphere $|\zeta|^2=\lambda$. This in turn implies that $\hat N_{\mathrm{sc}}(\Delta-\lambda)$ is not invertible, as discussed above. Incidentally, the argument we just described works even if g is an arbitrary scattering metric on $\mathbb{S}^N_+$ (but then, with $P=\Delta-\lambda$, $\tilde P\in\Psi^0(\mathbb{R}^N)$ is not necessarily just a multiplication operator), or indeed if X is an arbitrary compact manifold with boundary; in the latter case we need to identify X with $\mathbb{S}^N_+$ locally near some point p on ∂X, and correspondingly only the restriction of $\hat N_{\mathrm{sc}}(P)$ to a neighborhood of ${}^{\mathrm{sc}}T^*_pX$ is realized as a principal symbol of an element of $\Psi^0(\mathbb{R}^N)$.

Returning to the geometric setting, the lack of invertibility of $\hat N_{\mathrm{sc}}(\Delta-\lambda)$ implies that generalized eigenfunctions of $\Delta-\lambda$ need not be 'trivial', i.e. they are not necessarily in $\dot{\mathcal{C}}^\infty(X)$. They are certainly smooth in the interior of X since $\sigma_{\mathrm{sc},2}(\Delta-$

λ) is elliptic, but their behavior at ∂X is much more complicated. Just as for interior singularities, the failure of a distribution $u \in \mathcal{C}^{-\infty}(X)$ to be in $\dot{\mathcal{C}}^\infty(X)$, i.e. its 'singularities', can be measured by a wave front set, $\mathrm{WF}_{\mathrm{sc}}(u)$. Corresponding to the symbol maps of $\mathrm{Diff}_{\mathrm{sc}}(X)$, this consists of two parts: one part is an extension of the usual wave front set from the interior to give a subset of the cosphere bundle S^*X, the other part at the boundary is a subset of ${}^{\mathrm{sc}}T^*_{\partial X}X$. The first part describes the smoothness properties of u, the second part its decay properties at ∂X. Due to the ellipticity of $\sigma_{\mathrm{sc},2}(\Delta-\lambda)$, $(\Delta-\lambda)u = 0$ implies that $\mathrm{WF}_{\mathrm{sc}}(u) \subset {}^{\mathrm{sc}}T^*_{\partial X}X$.

The singularities of generalized eigenfunctions of $\Delta-\lambda$ were analyzed by Melrose in [22]. To facilitate this analysis, let x be the boundary defining function used in the definition of g, and let y_j be local coordinates on ∂X, extended to X. Then a covector $v \in {}^{\mathrm{sc}}T^*_pX$, p near ∂X, can be written as $v = \tau x^{-2}\,dx + \mu\cdot x^{-1}\,dy$. Hence, we have local coordinates (x, y, τ, μ) on ${}^{\mathrm{sc}}T^*X$ near ∂X. In these coordinates

$$\hat{N}_{\mathrm{sc}}(\Delta-\lambda) = \tau^2 + |\mu|^2 - \lambda; \tag{1.11}$$

here $|.|$ is the metric function of $h|_{\partial X}$. The characteristic set, $\Sigma_{\Delta-\lambda} \subset {}^{\mathrm{sc}}T^*_{\partial X}X$, of $\Delta-\lambda$ is the set where $\hat{N}_{\mathrm{sc}}(\Delta-\lambda)$ vanishes. Just as in the case of operators on compact manifolds without boundary, there is a (rescaled) Hamilton vector field associated to operators $P \in \mathrm{Diff}_{\mathrm{sc}}(X)$. Its restriction to ${}^{\mathrm{sc}}T^*_{\partial X}X$ is denoted by ${}^{\mathrm{sc}}H_p$, and it only depends on $p = \hat{N}_{\mathrm{sc}}(P)$. It is related to the commutator $[P,Q]$ for $P, Q \in \mathrm{Diff}_{\mathrm{sc}}(X)$. Indeed, $[P,Q] \in x\,\mathrm{Diff}_{\mathrm{sc}}(X)$, and $\hat{N}_{\mathrm{sc}}(x^{-1}[P,Q]) = \frac{1}{i}{}^{\mathrm{sc}}H_p q$. Correspondingly, as expected, ${}^{\mathrm{sc}}H_\lambda = 0$, and with g denoting the metric function on ${}^{\mathrm{sc}}T^*_{\partial X}X$, the Hamilton vector field of $\Delta-\lambda$ is just ${}^{\mathrm{sc}}H_g$. There are two disjoint submanifolds of $\Sigma_{\Delta-\lambda}$ where ${}^{\mathrm{sc}}H_g$ vanishes, namely

$$R^\pm_\lambda = \{(y,\tau,\mu) \in \Sigma_{\Delta-\lambda} : \ \mu = 0,\ \tau = \pm\lambda^{1/2}\}; \tag{1.12}$$

these are called 'radial surfaces'. The integral curves $\gamma(t)$ of ${}^{\mathrm{sc}}H_g$ approach $R^\pm_\lambda$ as $t \to \mp\infty$. The closure of the projection of each integral curve $\gamma(t)$ to ∂X gives a geodesic segment of $h|_{\partial X}$ of length π after reparametrization. Now, away from $R^\pm_\lambda$, where ${}^{\mathrm{sc}}H_g$ does not vanish, we have principal type propagation of singularities just as for hyperbolic operators on manifolds without boundary – in fact, we should think of $\Delta-\lambda$ as a hyperbolic operator at ∂X. Such a correspondence is made explicit by the Fourier transform if $X = \mathbb{S}^N_+$ is the radial compactification of $\mathbb{R}^N$, and by a localized version of the Fourier transform in the general case as described in the previous paragraphs. Just as in the standard case of manifolds without boundary, the propagation results can be obtained by positive commutator estimates; this is the significance of ${}^{\mathrm{sc}}H_g$. The singularities of the scattering matrix then correspond to singularities propagating from R^-_λ to R^+_λ along the bicharacteristics.

If we add a potential $V \in x\mathcal{C}^\infty(X)$ and consider $H-\lambda = \Delta+V-\lambda$, then $\hat{N}_{\mathrm{sc}}(H-\lambda) = \hat{N}_{\mathrm{sc}}(\Delta-\lambda)$, so in the region of principal type propagation the previous analysis applies; again, this is described in [22]. If, however, we consider $V \in \rho_{\mathrm{mf}}\mathcal{C}^\infty([X;C])$, then the behavior of commutators with H is radically changed. Thus, propagation of singularities for generalized eigenfunctions of H is very similar to the propagation phenomena in hyperbolic boundary and transmission problems, and the broken geodesics in the statement of the Theorem arise for similar reasons as the broken bicharacteristics in those cases. In fact, many of the proofs of those phenomena, such as those given by Hörmander in [16, Chapter XXIV], can be adapted to our setting.

Again, it may be of some use to relate certain parts of Melrose's analysis of the propagation of singularities to the standard form of Hörmander's theorem via the Fourier transform. Thus, in the Euclidian setting, $X = \mathbb{S}^N_+$, Δ the standard Laplacian, $P = \Delta - \lambda$, $\lambda > 0$, we have $\tilde{P} = \mathcal{F}P\mathcal{F}^{-1} = |\zeta|^2 - \lambda \in \Psi^0(\mathbb{R}^N_\zeta)$ with characteristic variety $\{(\zeta,\zeta^*) : \ |\zeta|^2 = \lambda\}$ (ζ^* is the cotangent variable). It is easy to see that the (non-rescaled) Hamilton vector field of $\tilde{P}$ is radial on the conormal bundle of the sphere given by $|\zeta|^2 = \lambda$, and its integral curves are straight lines in $T^*\mathbb{R}^N$ whose projection to the base variables (i.e., ζ) is constant. Indeed, projecting them to the cosphere bundle $S^*\mathbb{R}^N$ (realized, say, as the unit sphere subbundle of $T^*\mathbb{R}^N$), they become either open half great circles connecting the 'incoming' and 'outgoing' parts,

$$N^\pm_\lambda = \{(\zeta, \pm\zeta/|\zeta|) : \ |\zeta|^2 = \lambda\}, \tag{1.13}$$

of the cosphere bundle, or points in $N^\pm_\lambda$ (corresponding to the vector field being radial there); note that $N^\pm_\lambda = L(R^\pm_\lambda)$, L being the Legendre diffeomorphism as above. Hence, Hörmander's theorem for real principal type propagation applies in this situation: if $(\Delta - \lambda)u = 0$, then $\mathrm{WF}(\mathcal{F}u)$ either contains such a semicircle, or it is disjoint from it. Now,

$$L(\mathrm{WF}_{\mathrm{sc}}(u) \cap {}^{\mathrm{sc}}T^*_{\mathbb{S}^{N-1}}\mathbb{S}^N_+) = \mathrm{WF}(\mathcal{F}u), \tag{1.14}$$

corresponding to the analogous relationship between the indicial operator in the scattering calculus and the principal symbol map for standard pseudo-differential operators under conjugation by the Fourier transform. Hence, the propagation of singularities for $\mathcal{F}u$ in Hörmander's sense (here u is a generalized eigenfunction of $\Delta-\lambda$) implies the results on the propagation of $\mathrm{WF}_{\mathrm{sc}}(u)$ which were described in the previous paragraphs. Again, this analysis can be modified easily to accommodate two-body type scattering (by using a local Fourier transform if necessary), but the transposition of this argument to three-body scattering seems to be more complicated (see, however, [36] for a less comprehensive analysis of three-body scattering employing the Fourier transform).

We now describe the commutator constructions in somewhat more detail. First, we define a new algebra of differential operators on X which includes both $\mathrm{Diff}_{\mathrm{sc}}(X)$ and $\mathcal{C}^\infty([X;C])$. It is convenient to introduce some notation. The front face of the blown up space, $[X;C]$, is denoted by ff. Defining functions for ff and mf will be denoted by ρ_{ff} and ρ_{mf} respectively. The blow down map is written as

$$\beta : [X;C] \to X; \tag{1.15}$$

ρ_{mf} and ρ_{ff} can be chosen so that $\rho_{\mathrm{mf}}\rho_{\mathrm{ff}} = \beta^* x$. The inclusion of $\mathrm{Diff}_{\mathrm{sc}}(X)$ into the new algebra is supposed to preserve interesting analytical properties. We are thus led to define

$$\mathrm{Diff}_{3\mathrm{sc}}(X) = \mathcal{C}^\infty([X;C]) \otimes_{\mathcal{C}^\infty(X)} \mathrm{Diff}_{\mathrm{sc}}(X). \tag{1.16}$$

For reasons of brevity the notation does not include C on which $\mathrm{Diff}_{3\mathrm{sc}}(X)$ depends. Now, $\mathrm{Diff}_{3\mathrm{sc}}(X)$ is actually an algebra with respect to operator composition, since for $V \in \mathcal{V}_{\mathrm{sc}}(X)$, $f \in \mathcal{C}^\infty([X;C])$, we have $[V,f] = Vf \in \rho_{\mathrm{mf}}\mathcal{C}^\infty([X;C])$ as $\mathcal{V}_{\mathrm{sc}}(X)$ lifts to be a subset of $\rho_{\mathrm{mf}}\mathcal{V}_{\mathrm{b}}([X;C])$. In this paper we will microlocalize $\mathrm{Diff}_{3\mathrm{sc}}(X)$ by constructing the corresponding algebra of pseudo-differential operators, $\Psi^{\infty,-\infty}_{3\mathrm{sc}}(X)$.

This algebra, $\Psi_{3sc}^{\infty,-\infty}(X)$, will have several properties which are similar to the fibred cusp algebras defined by Mazzeo and Melrose in [20]. In fact, in the interior of ff, $\mathrm{Diff}_{3sc}(X)$ is a fibred cusp algebra (though on a non-compact manifold). Thus, many of the proofs are essentially adaptations of the proofs in [20], although in this paper we refrain from blowing up C on many occasions (thereby hiding the similarity), and only do the blow-ups necessary to obtain the b-fibrations required for push-forward results when the need arises.

One of the main differences between $\mathrm{Diff}_{3sc}(X)$ and $\mathrm{Diff}_{sc}(X)$ is that the former is not commutative to 'top weight'. That is, while for $P \in \mathrm{Diff}_{sc}^m(X)$, $Q \in \mathrm{Diff}_{sc}^{m'}(X)$, we have $[P,Q] \in x\,\mathrm{Diff}_{sc}^{m+m'-1}(X)$, this is replaced by $[P,Q] \in \rho_{\mathrm{mf}}\,\mathrm{Diff}_{3sc}^{m+m'-1}(X)$ for $P \in \mathrm{Diff}_{3sc}^m(X)$, $Q \in \mathrm{Diff}_{3sc}^{m'}(X)$. Thus, there is no gain of a weight factor at ff.

Now consider the operator $H = \Delta + V$, $V \in \rho_{\mathrm{mf}}\mathcal{C}^\infty([X;C])$, discussed above. As indicated in the previous paragraph, for $P \in \mathrm{Diff}_{sc}^m(X)$,

$$[\Delta, P] \in x\,\mathrm{Diff}_{sc}^{m+1}(X) \subset \rho_{\mathrm{mf}}\rho_{\mathrm{ff}}\,\mathrm{Diff}_{3sc}^{m+1}(X). \tag{1.17}$$

On the other hand,

$$[V, P] \in \rho_{\mathrm{mf}}^2\,\mathrm{Diff}_{3sc}^{m-1}(X). \tag{1.18}$$

Hence, as expected, $[V,P]$ is lower order than $[\Delta,P]$ at mf. However, at ff it can actually be higher order. That is, the term $[V,P]$ can dominate $[\Delta,P]$ there! This would clearly cause very serious problems for positive commutator arguments used, for example, to prove results on the propagation of singularities. We can avoid this by choosing P carefully. Thus, we take P from the 'symbolic center', $Z\,\mathrm{Diff}_{3sc}(X) \subset \mathrm{Diff}_{sc}(X)$ of $\mathrm{Diff}_{3sc}(X)$, i.e. we choose $P \in \mathrm{Diff}_{3sc}^m(X)$ so that $[P,Q] \in \rho_{\mathrm{mf}}\rho_{\mathrm{ff}}\,\mathrm{Diff}_{3sc}^{m+m'-1}(X)$ for all $Q \in \mathrm{Diff}_{3sc}^{m'}(X)$. This makes $[V,P]$ the same order as $[\Delta,P]$ with additional vanishing at mf which will be sufficient for the commutator arguments. While the leading part of $[V,P]$ can be quite complicated since it does depend on 'sub-leading' terms, the standard Poisson bracket formula lets us deal with $[\Delta,P]$ easily. The additional vanishing of $[V,P]$ at mf will ensure (due to compactness arguments) that relatively simple estimates of this commutator suffice.

The commutator approach we just outlined can give global positive estimates, such as the Mourre estimate, for $H = \Delta + V$. However, we need to introduce the corresponding pseudo-differential algebra, $\Psi_{3sc}^{\infty,-\infty}(X)$, for a microlocal description of the propagation of singularities at ∂X. These will propagate along broken bicharacteristics of ${}^{sc}H_g$, broken only at C, with the usual law of reflection satisfied at the 'break points'. The spreading of the singularities from a bicharacteristic to other ones when it hits C corresponds to the restriction in the choice of P in the commutator estimates mentioned above.

This paper consists of two major parts. In the first half we construct $\Psi_{3sc}^{\infty,-\infty}(X)$ and investigate its general properties. In the second half of the paper, starting with Section 11, we focus our attention on three-body type Hamiltonians and prove such results as the propagation of singularities for generalized eigenfunctions of these operators.

More specifically, in Section 2 we discuss some properties of the differential operator algebra $\mathrm{Diff}_{3sc}(X)$. Most of this section consists of a description of the indicial and normal operators for this algebra, since their behavior is significantly different from those for the scattering calculus. We define the microlocalization, $\Psi_{3sc}^{m,l}(X)$, of $\mathrm{Diff}_{3\mathrm{sc}}(X)$ in Section 3, and in the subsequent sections we analyze its properties, mostly following [20]. A more detailed plan of these sections is given at the beginning of Section 3.

In Section 11 we describe the basic properties of the Hamiltonian, $H = \Delta + V$. We then prove the Mourre estimate in our setting in Section 12; our method is very similar to Froese's and Herbst's in [8]. This could be used to analyze spectral properties of H, just as in Mourre's work [27], but we adopt instead the approach of [16, Chapter XXX] and [22]. We proceed to show in Sections 13-16 that singularities propagate along broken bicharacteristics of the (rescaled) Hamilton vector field, ${}^{\mathrm{sc}}H_g$, of g.

We continue in Section 17 by showing that H has no positive eigenvalues and in Section 18 we describe the boundary value of the resolvent at the real axis, $R(\lambda \pm i0)$, $\lambda > 0$, applied to $f \in \dot{\mathcal{C}}^\infty(X)$. This is basically the many-body result of of Gérard, Isozaki and Skibsted [9, 19] in our setting, with the additional microlocal variables included, together with the full asymptotic expansion away from C given in [35]. It should be noted that the propagation estimates of [9] correspond to microlocalization with respect to the operator $x^2 D_x$ only. This is completely sufficient for spectral theory, uniqueness statements, and (with slightly more involved arguments) for asymptotic expansions of $R(\lambda \pm i0)f$, $f \in \dot{\mathcal{C}}^\infty(X)$, but it cannot capture the singularities of the scattering matrix, for example.

We end the discussion by analyzing the scattering matrix in Section 19 using our results concerning the propagation of singularities and the plane wave construction of Melrose and Zworski [26] near the 'initial point' (the easy part of their construction, which we recall in Appendix A).

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