PROPAGATION OF SINGULARITIES IN MANY-BODY SCATTERING

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Abstract. In this paper we describe the propagation of singularities of tempered distributional solutions $u \in \mathcal{S}'$ of $(H-\lambda)u = 0$, $\lambda > 0$, where H is a many-body Hamiltonian $H = \Delta + V$, $\Delta \geq 0$, $V = \sum_a V_a$, under the assumption that no subsystem has a bound state and that the two-body interactions V_a are real-valued polyhomogeneous symbols of order -1 (e.g. Coulomb-type with the singularity at the origin removed). Here the term 'singularity' provides a microlocal description of the lack of decay at infinity. We use this result to prove that the wave front relation of the free-to-free S-matrix (which, under our assumptions, is all of the S-matrix) is given by the broken geodesic flow, broken at the 'singular directions', on $\mathbb{S}^{n-1}$ at time π. We also present a natural geometric generalization to asymptotically Euclidean spaces.

Propagation des singularités pour la diffusion dans le problème à N corps

Résumé. Dans cet article on décrit la propagation des singularités des solutions tempérées $u \in \mathcal{S}'$ de $(H-\lambda)u = 0$, $\lambda > 0$, où H est un Hamiltonien à N corps $H = \Delta + V$, $\Delta \geq 0$, $V = \sum_a V_a$, en supposant que les Hamiltoniens des sous-systèmes n'ont pas de vecteurs propres (dans L^2), et que les potentiels à deux corps V_a sont des symboles polyhomogènes réels d'ordre -1 (par exemple, de type Coulomb, mais sans la singularité à l'origine). Ici le terme "singularité" fournit une description microlocale de la croissance des fonctions à l'infini. On emploie ce résultat pour montrer que la relation de front d'onde de la matrice de diffusion, N-amas N-amas (qui est la seule partie de la matrice de diffusion sous nos hypothèses), est donnée par le flot géodesique brisé dans les "directions singulières", sur $\mathbb{S}^{n-1}$ à temps π. On présente aussi une généralisation géometrique naturelle au cas des variétés asymptotiquement euclidiennes.

1. Introduction

In this paper we describe the propagation of singularities of generalized eigenfunctions of a many-body Hamiltonian $H = \Delta + V$, Δ the *positive* Laplacian, under the assumption that no subsystem has a bound state. We use this result to prove that the wave front relation of the free-to-free S-matrix (which is the only part of the S-matrix under our assumptions) is given by the broken geodesic flow, broken at the 'singular directions', on $\mathbb{S}^{n-1}$ at distance π. We remark that these results have been proved in three-body scattering, without the assumption on the absence of bound states, in [36]. Also, Bommier [1] and Skibsted [33] have shown that the kernels of the 2-cluster to free cluster and 2-cluster to 2-cluster S-matrices are smooth,

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and previously Isozaki had showed this in the three-body setting [14]. However, as is clear from the smoothness statement, the microlocal propagation picture that is crucial, for instance, in the discussion of free-to-free scattering, does not emerge in the previous examples when the initial state is a 2-cluster.

In this section we discuss the setup in the Euclidean setting, but in the following ones we move to a natural geometric generalization introduced by Melrose in [22]. Namely, suppose that X is a manifold with boundary equipped with a scattering metric g and a cleanly intersecting family $\mathcal{C}$ of closed embedded submanifolds of ∂X with $C_0 = \partial X \in \mathcal{C}$. Thus, g is a Riemannian metric in $\mathrm{int}(X)$ which is of the form $g = x^{-4}\,dx^2 + x^{-2}h$ near ∂X; here $x \in \mathcal{C}^\infty(X)$ is a boundary defining function. We also assume that near every $p \in \partial X$, $\mathcal{C}$ is locally linearizable (i.e. in suitable coordinates near p, every element of $\mathcal{C}$ is linear); this holds if every element of $\mathcal{C}$ is totally geodesic with respect to some metric (not necessarily h) on ∂X. Let Δ be the positive Laplacian of g and suppose that $V \in \mathcal{C}^\infty([X;\mathcal{C}];\mathbb{R})$ vanishes at $\partial X \setminus \bigcup\{C \in \mathcal{C} :\ C \neq \partial X\}$, and $H = \Delta + V$ – we refer to Sections 2 and 6 for a more detailed discussion of the geometric and analytic aspects of the setup. We prove under the assumption that there are no bound states for each of the subsystems (we describe the assumption more precisely in Section 6, but it holds for example if $V \geq 0$) that singularities of solutions $u \in \mathcal{C}^{-\infty}(X)$ of $(H-\lambda)u \in \dot{\mathcal{C}}^\infty(X)$ propagate along generalized broken bicharacteristics of Δ which are broken at $\mathcal{C}$. We also show that this implies a bound on the singularities of the kernel of the free-to-free S-matrix. In effect, we show that many-body scattering is in many respects a hyperbolic problem, much like the wave equation in domains with corners, for which the propagation of analytic singularities was proved by Lebeau [18]. The geometrically simpler setting, where the elements of $\mathcal{C}$ (except $C_0 = \partial X$) are disjoint, corresponds to three-body scattering in the Euclidean setting, and then the analogy is with the wave equation in smoothly bounded domains, where the results for $\mathcal{C}^\infty$ singularities were proved by Melrose and Sjöstrand [23, 24] and Taylor [34], and for analytic singularities by Sjöstrand [32].

Here however we caution that another important aspect of typical many-body systems *is* the presence of bound states of subsystems. While propagation theorems indicate that geometry plays a central role in scattering, bound states afford a similar role to spectral theory. Thus, in general, the two interact, even changing the characteristic set of the Hamiltonian. The generalized broken bicharacteristics are also more complicated in this setting, and, as a quick argument shows, the 'time π' part of our result will not hold if bound states are present. In addition, the Hamiltonian must possess additional structure (as the Euclidean ones do) so that propagation in bound states can be analyzed. Hence, in this paper, it is natural to impose our assumption that there are no bound states in the subsystems.

We emphasize that this assumption holds, for example, if $V \geq 0$. Indeed, then $H = \Delta + V \geq 0$, and by an argument generalizing the corresponding result of Froese and Herbst [4] in the Euclidean setting, H has no positive eigenvalues. The proof of this fact in the geometric three-body setting can be found in [40], and it goes through in the geometric many-body setting since the potentials play a very minor role; they only enter via the Mourre estimate. Moreover, 0 cannot be an eigenvalue since for such an $L^2(dg)$ eigenfunction u, $0 = \langle (H+V)u, u\rangle = \|du\|_{L^2} + \langle u, Vu\rangle$, which implies that u is a constant, contradicting its L^2 behavior. (The argument is justified by elliptic regularity.)

We now return to the Euclidean setting. Before we can state the precise definitions, we need to introduce some basic (and mostly standard) notation. We consider the Euclidean space $\mathbb{R}^n$, and we assume that we are given a (finite) family $\mathcal{X}$ of linear subspaces X_a, $a \in I$, of $\mathbb{R}^n$ which is closed under intersections and includes the subspace $X_1 = \{0\}$ consisting of the origin, and the whole space $X_0 = \mathbb{R}^n$. Let X^a be the orthocomplement of X_a, and let π^a be the orthogonal projection to X^a, π_a to X_a. A many-body Hamiltonian is an operator of the form

$$H = \Delta + \sum_{a \in I} (\pi^a)^* V_a; \tag{1.1}$$

here Δ is the positive Laplacian, $V_0 = 0$, and the V_a are real-valued functions in an appropriate class which we take here to be polyhomogeneous symbols of order -1 on the vector space X_a to simplify the problem:

$$V_a \in S^{-1}_{\mathrm{phg}}(X^a). \tag{1.2}$$

In particular, smooth potentials V_a which behave at infinity like the Coulomb potential are allowed. Since $(\pi^a)^* V_a$ is bounded and self-adjoint and Δ is self-adjoint with domain $H^2(\mathbb{R}^n)$ on $L^2 = L^2(\mathbb{R}^n)$, H is also a self-adjoint operator on L^2 with domain $H^2(\mathbb{R}^n)$. We let $R(\lambda) = (H - \lambda)^{-1}$ for $\lambda \in \mathbb{C} \setminus \mathbb{R}$ be the resolvent of H.

There is a natural partial ordering on I induced by the ordering of X^a by inclusion. (Though the ordering based on inclusion of the X_a would be sometimes more natural, and we use that for the geometric generalization of many-body scattering starting from the next section, here we use the conventional ordering.) Let $I_1 = \{1\}$ (recall that $X_1 = \{0\}$); 1 is the maximal element of I. A maximal element of $I \setminus I_1$ is called a 2-cluster; I_2 denotes the set of 2-clusters. In general, once I_k has been defined for $k = 1, \ldots, m-1$, we let I_m (the set of m-clusters) be the set of maximal elements of $I'_m = I \setminus \cup_{k=1}^{m-1} I_k$, if I'_m is not empty. If $I'_m = \{0\}$ (so I'_{m+1} is empty), we call H an m-body Hamiltonian. For example, if $I \neq \{0, 1\}$, and for all $a, b \notin \{0, 1\}$ with $a \neq b$ we have $X_a \cap X_b = \{0\}$, then H is a 3-body Hamiltonian. The N-cluster of an N-body Hamiltonian is also called the free cluster, since it corresponds to the particles which are asymptotically free.

It is convenient to compactify these spaces as in [22]. Thus, we let $\mathbb{S}^n_+$ to be the radial compactification of $\mathbb{R}^n$ to a closed hemisphere, i.e. a ball, (using the standard map RC given here in (2.3)), and $\mathbb{S}^{n-1} = \partial \mathbb{S}^n_+$. We write $w = r\omega$, $\omega \in \mathbb{S}^{n-1}$, for polar coordinates on $\mathbb{R}^n$, and we let $x \in \mathcal{C}^\infty(\mathbb{S}^n_+)$ be such that $x = (\mathrm{RC}^{-1})^*(r^{-1})$ for $r > 1$. Hence, x is a smoothed version of r^{-1} (smoothed at the origin of $\mathbb{R}^n$), and it is a boundary defining function of $\mathbb{S}^n_+$. We usually identify (the interior of) $\mathbb{S}^n_+$ with $\mathbb{R}^n$. Thus, we write $S^m_{\mathrm{phg}}(\mathbb{S}^n_+)$ and $S^m_{\mathrm{phg}}(\mathbb{R}^n)$ interchangeably and we drop the explicit pull-back notation in the future and simply write $x = r^{-1}$ (for $r > 1$). We also remark that we have

$$S^m_{\mathrm{phg}}(\mathbb{S}^n_+) = x^m \mathcal{C}^\infty(\mathbb{S}^n_+). \tag{1.3}$$

We recall that under RC, $\dot{\mathcal{C}}^\infty(\mathbb{S}^n_+)$, the space of smooth functions on $\mathbb{S}^n_+$ vanishing to infinite order at the boundary corresponds to the space of Schwartz functions $\mathcal{S}(\mathbb{R}^n)$, and its dual, $\mathcal{C}^{-\infty}(\mathbb{S}^n_+)$, to tempered distributions $\mathcal{S}'(\mathbb{R}^n)$. We also have the following correspondence of weighted Sobolev spaces

$$H^{k,l}_{\mathrm{sc}}(\mathbb{S}^n_+) = H^{k,l} = H^{k,l}(\mathbb{R}^n) = \langle w \rangle^{-l} H^k(\mathbb{R}^n) \tag{1.4}$$

where $\langle w\rangle = (1+|w|^2)^{1/2}$. Thus, for $\lambda \in \mathbb{C}\setminus\mathbb{R}$ the resolvent extends to a map

$$R(\lambda) : H^{k,l}_{\mathrm{sc}}(\mathbb{S}^n_+) \to H^{k+2,l}_{\mathrm{sc}}(\mathbb{S}^n_+). \tag{1.5}$$

Similarly, we let

$$\bar{X}_a = \mathrm{cl}(\mathrm{RC}(X_a)), \quad C_a = \bar{X}_a \cap \partial\mathbb{S}^n_+. \tag{1.6}$$

Hence, C_a is a sphere of dimension $n_a - 1$ where $n_a = \dim X_a$. We also let

$$\mathcal{C} = \{C_a : \ a \in I\}. \tag{1.7}$$

Again, we write the polar coordinates on X_a (with respect to the induced metric) as $w_a = r_a\omega_a$, $\omega_a \in C_a$, and let $x_a = r_a^{-1}$ (for $r_a > 1$). We note that if a is a 2-cluster then $C_a \cap C_b = \emptyset$ unless $b \le a$. We also define the 'singular part' of C_a as the set

$$C_{a,\mathrm{sing}} = \cup_{b \not\leq a}(C_b \cap C_a), \tag{1.8}$$

and its 'regular part' as the set

$$C'_a = C_a \setminus \cup_{b\not\leq a} C_b = C_a \setminus C_{a,\mathrm{sing}}. \tag{1.9}$$

For example, if a is a 2-cluster then $C_{a,\mathrm{sing}} = \emptyset$ and $C'_a = C_a$. We sometimes write the coordinates on $X_a \oplus X^a$ as (w_a, w^a).

Corresponding to each cluster a we introduce the cluster Hamiltonian h_a as an operator on $L^2(X^a)$ given by

$$h_a = \Delta + \sum_{b\le a} V_b, \tag{1.10}$$

Δ being the Laplacian of the induced metric on X^a. Thus, if H is a N-body Hamiltonian and a is a k-cluster, then h_a is a $(N+1-k)$-body Hamiltonian. The L^2 eigenfunctions of h_a play an important role in many-body scattering; we remark that by Froese's and Herbst's result, [4], $\mathrm{spec}_{pp}(h_a) \subset (-\infty, 0]$ (there are no positive eigenvalues). Moreover, $\mathrm{spec}_{pp}(h_a)$ is bounded below since h_a differs from Δ by a bounded operator. Note that $X^0 = \{0\}$, $h_0 = 0$, so the unique eigenvalue of h_0 is 0.

The eigenvalues of h_a can be used to define the set of thresholds of h_b. Namely, we let

$$\Lambda_a = \cup_{b<a} \mathrm{spec}_{pp}(h_b) \tag{1.11}$$

be the set of thresholds of h_a, and we also let

$$\Lambda'_a = \Lambda_a \cup \mathrm{spec}_{pp}(h_a) = \cup_{b\le a} \mathrm{spec}_{pp}(h_b). \tag{1.12}$$

Thus, $0 \in \Lambda_a$ for $a \neq 0$ and $\Lambda_a \subset (-\infty, 0]$. It follows from the Mourre theory (see e.g. [5, 27]) that Λ_a is closed, countable, and $\mathrm{spec}_{pp}(h_a)$ can only accumulate at Λ_a. Moreover, $R(\lambda)$, considered as an operator on weighted Sobolev spaces, has a limit

$$R(\lambda \pm i0) : H^{k,l}_{\mathrm{sc}}(\mathbb{S}^n_+) \to H^{k+2,l'}_{\mathrm{sc}}(\mathbb{S}^n_+) \tag{1.13}$$

for $l > 1/2$, $l' < -1/2$, from either half of the complex plane away from

$$\Lambda = \Lambda_1 \cup \mathrm{spec}_{pp}(H). \tag{1.14}$$

In addition, L^2 eigenfunctions of h_a with eigenvalues which are not thresholds are necessarily Schwartz functions on X^a (see [4]). We also label the eigenvalues of h_a, counted with multiplicities, by integers m, and we call the pairs $\alpha = (a, m)$ channels.

We denote the eigenvalue of the channel α by ϵ_α, write ψ_α for a corresponding normalized eigenfunction, and let e_α be the orthogonal projection to ψ_α in $L^2(X^a)$.

The definition of the free-to-free S-matrix we consider comes from the stationary theory, more precisely from the asymptotic behavior of generalized eigenfunctions, see [35], and cf. [22, 40]. Apart from the difference in normalization, it is the same as the S-matrix given by the wave operators, see [39]. For simplicity, we state the asymptotic expansion under the assumption that V_a is polyhomogeneous of order -2 (so it decays as $|w^a|^{-2}$). Namely, for $\lambda \in (0,\infty)$ and $g \in \mathcal{C}_c^\infty(C_0')$, there is a unique $u \in \mathcal{C}^{-\infty}(\mathbb{S}^n_+)$ (i.e. $u \in \mathcal{S}'(\mathbb{R}^n)$) such that $(H-\lambda)u = 0$, and u has the form

$$u = e^{-i\sqrt{\lambda}r} r^{-(n-1)/2} v_- + R(\lambda + i0)f, \tag{1.15}$$

where $v_- \in \mathcal{C}^\infty(\mathbb{S}^n_+)$, $v_-|_{\mathbb{S}^{n-1}} = g$, and $f \in \dot{\mathcal{C}}^\infty(\mathbb{S}^n_+)$. In addition, this u is of the form

$$u = e^{-i\sqrt{\lambda}r} r^{-(n-1)/2} v_- + e^{i\sqrt{\lambda}r} r^{-(n-1)/2} v_+, \quad v_+ \in \mathcal{C}^\infty(\mathbb{S}^n_+ \setminus C_{0,\mathrm{sing}}). \tag{1.16}$$

The Poisson operator with free initial data is the operator

$$P_{0,+}(\lambda) : \mathcal{C}_c^\infty(C_0') \to \mathcal{C}^{-\infty}(\mathbb{S}^n_+), \quad P_{0,+}(\lambda)g = u. \tag{1.17}$$

Following [35], we define the free-to-free scattering matrix, $S_{00}(\lambda)$ as the map

$$S_{00}(\lambda) : \mathcal{C}_c^\infty(C_0') \to \mathcal{C}^\infty(C_0'), \tag{1.18}$$

$$S_{00}(\lambda)g = v_+|_{C_0'}, \tag{1.19}$$

so it relates the incoming amplitude $v_-|_{\mathbb{S}^{n-1}}$ to the outgoing one, $v_+|_{\mathbb{S}^{n-1}}$. We recall from [39] that the wave operator free-to-free S-matrix is then given by $i^{n-1}S_{00}(\lambda)R$ (as maps $\mathcal{C}_c^\infty(C_0') \to \mathcal{C}^{-\infty}(C_0')$) where R is pull back by the antipodal map on C_0.

There are only minor changes if V_a is polyhomogeneous of order -1. Namely, the asymptotic expansions in (1.15) and (1.16) must be replaced by

$$e^{\pm i\sqrt{\lambda}r} r^{-i\alpha_\pm - (n-1)/2} v_\pm, \quad \alpha_\pm = \alpha_{\pm,\lambda} = \pm V'|_{C_0'}/2\sqrt{\lambda} \in \mathcal{C}^\infty(C_0'),\ V = xV', \tag{1.20}$$

$$v_\pm \sim \sum_{j=0}^\infty \sum_{s \le 2j} a_{j,s,\pm}(\omega) r^{-j} (\log r)^s, \quad a_{j,s,-} \in \mathcal{C}_c^\infty(C_0'),\ a_{j,s,+} \in \mathcal{C}^\infty(C_0'). \tag{1.21}$$

Note that $\alpha_\pm$ are not defined at $C_{0,\mathrm{sing}}$, but that does not cause any problems even in the uniqueness statement, (1.15), since v_- vanishes at $\mathbb{S}^{n-1}$ near $C_{0,\mathrm{sing}}$ to infinite order.

Our main theorem describes the structure of $S_{00}(\lambda)$. We first introduce the broken geodesic flow (of the standard Riemannian metric h) on $\mathbb{S}^{n-1}$, broken at $\mathcal{C}$. We denote by $S\mathbb{S}^{n-1}$ the sphere bundle of $\mathbb{S}^{n-1}$ identified as the unit-length subbundle of $T\mathbb{S}^{n-1}$ with respect to h. Let $I = [\alpha, \beta] \subset \mathbb{R}$ be an interval. We say that a curve $\gamma : I \to \mathbb{S}^{n-1}$ is a broken geodesic of h, broken at $\mathcal{C}$, if two conditions are satisfied. First, there exists a finite set of points $t_j \in I$, $\alpha = t_0 < t_1 < \ldots < t_{k-1} < t_k = \beta$ such that for each j, $\gamma|_{[t_j, t_{j+1}]}$ is a geodesic of h, and for all $t \in (t_j, t_{j+1})$, $\gamma'(t) \in S\mathbb{S}^{n-1}$. Second, for all j, if $\gamma(t_j) \in C_a'$ then the limits $\gamma'(t_j - 0)$ and $\gamma'(t_j + 0)$ both exist and differ by a vector in $T_{\gamma(t_j)}\mathbb{S}^{n-1}$ which is orthogonal to $T_{\gamma(t_j)}C_a$ (i.e. the usual law of reflection is satisfied; see Figure 1). We say that $p, q \in S\mathbb{S}^{n-1}$ are related by the broken geodesic flow at time π if there is a broken geodesic γ defined on $[0, \pi]$, 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 π on $S^*\partial X$. We refer to Definition 6.6 and Section 7 for a more complete discussion. We then have the following result:

Theorem. *Suppose that no subsystem of H has bound states, i.e. for $a \neq 0$, $\operatorname{spec}_{pp}(h_a) = \emptyset$. Then the free-to-free scattering matrix, $S_{00}(\lambda)$, extends to a continuous linear map $\mathcal{C}_c^{-\infty}(C_0') \to \mathcal{C}^{-\infty}(C_0')$. The wave front relation of $S_{00}(\lambda)$ is given by the broken geodesic flow at time π.*

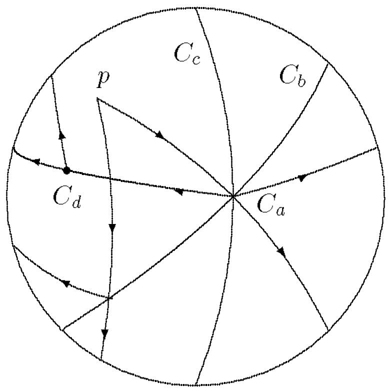

FIGURE 1. Broken geodesics on $\mathbb{S}^2$ starting at p. Here $C_a = C_b \cap C_c$.

In the actual many-body problem, $w \in X_a$ means that several particles are close to each other, namely the ones corresponding to the cluster decomposition a. Thus, $\omega \in C_a$ is a statement that the particles corresponding to cluster a collide. Hence, the Theorem describes how many-body scattering can be understood, modulo smoothing (hence in the $\mathcal{C}^\infty$ sense trivial) terms, as a sequence of a finite number of collisions involving the particles. Namely, each 'break' t_j in the broken geodesic describes a collision involving the cluster decomposition a. In the three-body setting with Schwartz potentials it was shown in [37] that the amplitude of the reflected wave is given, to top order, by the corresponding 2-body S-matrix; an analogous statement also holds for short-range potentials. In particular, this shows that the Theorem is sharp as far as the location of singularities is concerned.

We also remark that in the Euclidean setting, unbroken geodesic flow to distance π amounts to pull-back by the antipodal map on $\mathbb{S}^{n-1} = \partial\mathbb{S}^n_+$, so it corresponds to free propagation: particles leave in the direction opposite to the one from which they entered.

Our approach to proving this theorem is via the analysis of generalized eigenfunctions of H, i.e. of $u \in \mathcal{C}^{-\infty}(\mathbb{S}^n_+)$ satisfying $(H - \lambda)u = 0$. We prove that 'singularities' of generalized eigenfunctions of H propagate along broken bicharacteristics in the characteristic set of H, similarly to singularities of the solutions of the wave equation. Here 'singularities' are not understood as the lack of smoothness: indeed H is elliptic in the usual sense, so every generalized eigenfunction is $\mathcal{C}^\infty$ in the interior of $\mathbb{S}^n_+$, i.e. on $\mathbb{R}^n$. Instead, in this situation singularity means the lack of rapid decay u. Correspondingly, we define a wave front set, $\mathrm{WF}_{\mathrm{Sc}}(u)$, at infinity, i.e. at $\partial\mathbb{S}^n_+$, and we will prove its invariance under the broken bicharacteristic flow.

The two notions of singularities are very closely related via the Fourier transform. Here for simplicity consider $\Delta - \lambda$ in place of $H - \lambda$. If $(\Delta - \lambda)u = 0$, then the Fourier transform of u, $\mathcal{F}u$, satisfies $(|\xi|^2 - \lambda)\mathcal{F}u = 0$ where ξ is the dual variable of w. Now, the multiplication operator $P = |\xi|^2 - \lambda$ can be regarded as a 0th order differential operator. Hence, by Hörmander's theorem, see e.g. [12], $\mathrm{WF}(\mathcal{F}u)$ is invariant under the bicharacteristic flow in the characteristic variety of P, i.e. in the set $\{(\xi, \xi^*) : \ |\xi|^2 - \lambda = 0\}$ where we have written ξ^* for the dual variable of ξ, so ξ^* is in fact w. Moreover, in the two-body problem, i.e. if V is a symbol (of say order -1) on $\mathbb{R}^n$, $H = \Delta + V$, and if $(H - \lambda)u = 0$, we still have $P\mathcal{F}u = 0$ where now $P = |\xi|^2 - \lambda + \mathcal{F}V\mathcal{F}^{-1}$. Since V is a symbol of order -1, $\mathcal{F}V\mathcal{F}^{-1}$ is a pseudo-differential operator of order -1, hence lower order than $|\xi|^2 - \lambda$. Thus, the principal symbol of P is still $|\xi|^2 - \lambda$ (recall that ξ^* is the cotangent variable, so this is indeed homogeneous of order 0 in ξ^* – it is independent of ξ^*). Hence, Hörmander's theorem is applicable and we have the same propagation statement as before.

In the two-body setting the relevant wave front set measuring lack of decay at infinity is the scattering one, $\mathrm{WF}_{\mathrm{sc}}$. For $u \in \mathcal{S}'(\mathbb{R}^n)$, $\mathrm{WF}_{\mathrm{sc}}(u)$ is essentially given by the usual wave front set of the Fourier transform of u, i.e. by $\mathrm{WF}(\mathcal{F}u)$, after interchanging the role of the base and dual variables. Since the Fourier transform interchanges decay at infinity and smoothness, $\mathrm{WF}(\mathcal{F}u)$ indeed measures the decay of u at infinity in a microlocal sense. Hence, Hörmander's propagation theorem translated directly into a propagation theorem for $\mathrm{WF}_{\mathrm{sc}}(u)$. This result was described by Melrose in [22] where he introduced the notion of $\mathrm{WF}_{\mathrm{sc}}$.

In the many-body setting conjugation by the Fourier transform is much less convenient. Hence, we will design an appropriate microlocal way of measuring the lack of decay at infinity without resorting to the Fourier transform. Instead, we introduce an algebra of many-body pseudo-differential operators $\Psi_{\mathrm{Sc}}(\mathbb{S}^n_+, \mathcal{C})$ which reflects the geometry, and use it to define the wave front set at infinity. We remark, however, that for (approximate) generalized eigenfunctions of H, a characterization based on the Fourier transform is possible; see Remark 5.3 and Proposition 5.5. We then prove a propagation of singularities theorem for generalized eigenfunctions of many-body Hamiltonians H; here 'singularities' are understood in the sense of the new wave front set at infinity. The proof of this theorem is via a microlocal positive commutator estimate, similarly to the proof of Hörmander's theorem, or indeed to the proof of the propagation theorems for $\mathcal{C}^\infty$ singularities of solutions of the wave equation with domains with boundaries [23]. Finally, we relate such a result to the structure of the S-matrix. This step is comparatively easy as indicated by our description of the S-matrix in terms of generalized eigenfunctions of H.

Positive commutator estimates have also played a major role in many-body scattering starting with the work of Mourre [26], Perry, Sigal and Simon [27], Froese and Herbst [5], Jensen [17], Gérard, Isozaki and Skibsted [6, 7] and Wang [41]. In particular, the Mourre estimate is one of them; it estimates $i[H, w \cdot D_w + D_w \cdot w]$. This and some other *global* positive commutator results have been used to prove the global results mentioned in the first paragraph about some of the S-matrices with initial state in a two-cluster. They also give the basis for the existence, uniqueness and equivalence statements in our definition of the S-matrix by asymptotic expansions; these statements are discussed in [39] in more detail. Correspondingly, these global estimates will appear in Sections 11-12 of this paper where we turn the propagation results for generalized eigenfunctions into statements about the S-matrix.

We remark that the wave-operator approach defines the S-matrix as a bounded operator $L^2(C_0) \to L^2(C_0)$. Since $C_{0,\mathrm{sing}}$ has measure 0, $L^2(C_0)$ and $L^2(C_0')$ can be identified. As $\mathcal{C}_c^\infty(C_0')$ is dense in $L^2(C_0')$, the asymptotic expansion S-matrix $S_{00}(\lambda)$ indeed determines the wave-operator one.

The propagation of singularities of generalized eigenfunctions of H is determined by the principal part of H; terms decaying at the boundary do not change the analysis. As opposed to this, the precise structure of incoming and outgoing functions, $R(\lambda \pm i0)f$, $f \in \dot{\mathcal{C}}^\infty(\mathbb{S}^n_+)$, depends on lower order terms; a relatively trivial example is given by the appearence of $r^{-i\alpha_\pm}$ in (1.20) for long-range potentials. Since we consider $S_{00}(\lambda)$ and $P_{0,+}(\lambda)$ as operators on distributions supported away from $C_{0,\mathrm{sing}}$, we do not need to analyze the precise structure of incoming/outgoing functions at $C_{0,\mathrm{sing}}$, which is not 'principal type', although we certainly analyze the propagation of singularities there. Thus, we do not discuss what happens when the support of the incoming scattering data increases to C_0', even if the data are L^2. But the behavior of $P_{0,+}(\lambda)$, as the support of the data increases to C_0', plays an important part in asymptotic completeness, which states that all possible outcomes of a scattering experiment are indeed described by a combination of bound states of the cluster Hamiltonians, with asymptotically free motion in the intercluster variables. Thus, our results cannot be used directly to supply a proof of asymptotic completeness. This completeness property of many-body Hamiltonians was proved by Sigal and Soffer, Graf, Dereziński and Yafaev under different assumptions on the potentials and by different techniques [28, 29, 31, 30, 8, 2, 42]. In particular, Yafaev's paper [42] shows quite explicitly the importance of the special structure of the Euclidean Hamiltonian. This structure enables him to obtain a positive commutator estimate, which would not follow from our indicial operator arguments in Section 9, and which is then used to prove asymptotic completeness.

Finally we comment on the requirement that the collection $\mathcal{C}$ be locally linearizable. We show in the next section that it is equivalent to the existence of a neighborhood of every point $p \in \partial X$ and a metric on it, in terms of which all elements of $\mathcal{C}$ are totally geodesic. The importance of this assumption is closely related to the existence of a sufficient number of *smooth* vector fields on ∂X which are tangent to every element of $\mathcal{C}$. Such smooth vector fields always exists once we *resolve* the geometry of $\mathcal{C}$, i.e. on the blown-up space $[\partial X; \mathcal{C}]$, but in general, without our assumption, there are not enough such smooth vector fields on ∂X. In the first part of the paper, we discuss the pseudo-differential algebra associated to many-body scattering. For this purpose we need to blow up $\mathcal{C}$, in part for analyzing the indicial operators (see the following paragraph). Thus, in this part of the paper, the issue of local linearizability is irrelevant, and we do not assume it. However, in the second part of the paper, the geometry of the compressed cotangent bundle, the discussion of generalized broken bicharacteristics and the construction of the positive commutators would all be more complicated without it, so from Section 5 on, we assume the local linearizability of $\mathcal{C}$.

This paper is organized as follows. In the next section we describe the geometric generalization of the many-body problem which was outlined above. This includes a discussion of many-body geometry and the definition of many-body differential operators. In Section 3 we proceed to define and analyze the corresponding algebra of pseudo-differential operators, $\Psi_{\mathrm{Sc}}(X, \mathcal{C})$, which reflects this geometry. It includes many-body Hamiltonians, as well as their resolvent away from the real axis. It extends the definition of the three-body calculus presented in [40], though here we emphasize the definition of the calculus via localization and quantization as opposed to the conormal description of the kernels on an appropriate resolved space. In Section 4 we construct the indicial operators in this calculus. They provide a non-commutative analog of the principal symbol in standard microlocal analysis. Our proof of positivity in commutator estimates is based on replacing the argument of Froese and Herbst [5] by indicial operator techniques. In Section 5 we define the wave front set at infinity, $\mathrm{WF}_{\mathrm{Sc}}(u)$, corresponding to the many-body geometry and pseudo-differential operators. The definition given here differs from the one in [40]; it follows the fibred cusp definition of Mazzeo and Melrose [19]. These definitions, however, give the same result for approximate generalized eigenfunctions of H.

In Section 6 we discuss many-body type Hamiltonians and their generalized broken bicharacteristics. This section is, to a significant degree, based on Lebeau's paper [18]. In Section 7 we give a much more detailed description of the generalized broken bicharacteristics in the case when all elements $C \in \mathcal{C}$ are totally geodesic. Of course, this is true in the Euclidean setting. In Sections 8-9 we build the technical tools for turning a symbolic positive commutator calculation into an operator estimate. In Section 10 we prove that singularities of generalized eigenfunctions of many-body type Hamiltonians propagate along generalized broken bicharacteristics. This is the main new result of the paper. In Sections 11-12 we use this and adaptations of the global estimates, in particular those of Gérard, Isozaki and Skibsted [6, 7], to analyze the structure of the resolvent and that of the scattering matrix. Finally, in the Appendix we prove some of the results quoted from Lebeau's paper, using slightly different methods.

The propagation estimates of Section 10 lie at the heart of this paper. The reader may want to skip some of the technical sections when reading the paper for the first time. It may be useful to keep Mourre-type estimates and especially their microlocalized versions as in [6, 7] in mind while reading Section 10.

I would like to thank Richard Melrose for suggesting this problem to me (in the three-body setting) as my PhD thesis problem and for our very fruitful discussions. His firm belief that scattering theory can be understood in microlocal terms similar to the well-known theory of hyperbolic operators motivated me both during my PhD work [36] and while working on its extension that appears in this paper. I am grateful to Maciej Zworski for introducing me to the work of Gilles Lebeau [18], for many helpful discussions and for his encouragement. It was Lebeau's paper that convinced me that the results presented here were within reach, and it plays a particularly central role in Section 6 where the generalized broken bicharacteristics are described. I would also like to thank the referee for the careful reading of the original mansucript and for the resulting numerous improvements. I am also grateful to Andrew Hassell, Rafe Mazzeo, Erik Skibsted and Jared Wunsch for helpful discussions, their encouragement and for their interest in this research.

2. Many-body geometry and differential operators

It is convenient to carry out the construction in the general geometric setting. We first describe the many-body geometry.

Thus, let X be a compact manifold with boundary, and let

$$\mathcal{C} = \{C_a : \ a \in I\} \tag{2.1}$$