PROPAGATION OF SINGULARITIES IN MANY-BODY SCATTERING IN THE PRESENCE OF BOUND STATES

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Abstract. In these lecture notes we describe the propagation of singularities of tempered distributional solutions $u \in \mathcal{S}'$ of $(H-\lambda)u = 0$, where H is a many-body Hamiltonian $H = \Delta + V$, $\Delta \geq 0$, $V = \sum_a V_a$, and λ is not a threshold of H, under the assumption that the inter-particle (e.g. 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. Our result is then that the set of singularities of u is a union of maximally extended broken bicharacteristics of H. These are curves in the characteristic variety of H, which can be quite complicated due to the existence of bound states. We use this result to describe the wave front relation of the S-matrices. Here we only present the statement of the results and sketch some of the ideas in proving them, the complete details will appear in [30].

1. Introduction

In these lecture notes we describe the propagation of singularities of generalized eigenfunctions of a many-body Hamiltonian $H = \Delta + V$, $V = \sum_a V_a$, on $\mathbb{R}^n$ under the assumption that the inter-particle interactions V_a are real-valued polyhomogeneous symbols of order -1 (e.g. Coulomb-type with the singularity at the origin removed). More precisely, we use the 'many-body scattering wave front set' $\mathrm{WF}_{\mathrm{Sc}}(u)$ at infinity for tempered distributions $u \in \mathcal{S}'(\mathbb{R}^n)$, and show that for $u \in \mathcal{S}'(\mathbb{R}^n)$ satisfying $(H-\lambda)u = 0$, $\mathrm{WF}_{\mathrm{Sc}}(u)$ is a union of maximally extended generalized broken bicharacteristics of H, broken at the collision planes. Here $\mathrm{WF}_{\mathrm{Sc}}(u)$ provides a microlocal description of the lack of decay of u modulo $\mathcal{S}(\mathbb{R}^n)$, similarly to how the usual wave front set describes distributions modulo $\mathcal{C}^\infty$ functions.

The definition of generalized broken bicharacteristics is quite technical due to the presence of bound states in the subsystems. However, if these bound states are absent, our definition becomes completely analogous to Lebeau's definition [17] for the wave equation in domains with corners. Indeed, in this case the propagation result itself, which was proved in [31], is a direct ($\mathcal{C}^\infty$-type) analogue of Lebeau's result for the propagation of analytic singularities for solutions of the wave equation in domains with corners.

If there are bound states in the subsystems, but either the set of thresholds is discrete, or H is a four-body Hamiltonian, the geometry of generalized broken bicharacteristics is not much more complicated than in Lebeau's setting. The general definition reflects that when particles collide, the total energy as well as the external momentum is preserved. The complication in the presence of bound states

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Partially supported by NSF grant #DMS-99-70607.

is that kinetic energy is not preserved, even asymptotically. In summary, our results provide a connection between quantum and classical objects, just as Lebeau's results connect the wave equation and geometric optics.

We also state the corresponding result in the 'limiting absorption principle' setting, namely that under certain assumptions on $\mathrm{WF}_{\mathrm{Sc}}(f)$, $R(\lambda \pm i0)f$ are defined, and $\mathrm{WF}_{\mathrm{Sc}}(R(\lambda + i0)f)$ is a subset of the image of $\mathrm{WF}_{\mathrm{Sc}}(f) \cup R_-(\lambda)$ under the forward broken bicharacteristic relation. Here $R_-(\lambda)$ is the outgoing 'radial set'. Such a result makes the 'radial-variable' propagation estimates that have been used in many-body scattering, especially as derived in the works of Gérard, Isozaki and Skibsted [6, 7], more precise.

We use this result to analyze that the wave front relation of the scattering matrices (S-matrices). These connect the incoming and outgoing data of generalized eigenfunctions of H, so one expects that their singularities are described by considering the limit points of generalized broken bicharacteristics $\gamma = \gamma(t)$ as $t \to \pm\infty$. In fact, in addition to the propagation of singularities result, the only ingredient that is required for this analysis is a good approximation for the incoming Poisson operators with incoming state α near the incoming region, and similar results for the outgoing Poisson operators with, say, outgoing state β. In general, one expects a WKB-type construction, essentially as in Hadamard's parametrix construction. Indeed, this is what Melrose and Zworski do in the geometric two-body type setting, [21]. In the Euclidean many-body setting this construction has been done by Skibsted [28] in the short-range and by Bommier [1] in the long-range setting, in the latter case by adopting the construction of Isozaki and Kitada [15], at least under the assumption that the energies of the states α, β are below the continuous spectrum of the corresponding subsystem Hamiltonians. Such a construction is unnecessary if V_c are Schwartz, for then the product decomposition is sufficiently accurate to give a good approximation for the Poisson operator. We thus obtain the following result.

Theorem. *Suppose that H is a many-body Hamiltonian, and λ is not a threshold or (L^2-)eigenvalue of H. Suppose also that either α and β are channels such that the corresponding eigenvalues ϵ_α, ϵ_β, of the subsystem Hamiltonians h_a, h_b, are in the discrete spectrum of h_a and h_b respectively, or that V_c is Schwartz for all c. Then the wave front relation of the S-matrix $S_{\beta\alpha}(\lambda)$, is given by the generalized broken bicharacteristic relation of H as stated precisely below in Theorem 2.8.*

Special cases, which have already been analyzed, include the free-to-free S-matrix in three-body scattering [29, 9, 33], or indeed in many-body scattering under the additional assumption that there are no bound states in any subsystem [31]. In these cases the wave front relation is given by the broken geodesic relation, broken at the collision planes, on $\mathbb{S}^{n-1}$ at distance π. In both cases, one can naturally extend the results to geometric many-body type problems on asymptotically Euclidean manifolds.

Also, Bommier [1] and Skibsted [28] have shown that the kernels of the 2-cluster to free cluster and 2-cluster to 2-cluster S-matrices are smooth (except for the diagonal singularity if the 2-clusters are the same), and previously Isozaki had showed this in the three-body setting [12]. We remark that (under our polyhomogeneous assumption) the proofs of Bommier and Skibsted in fact show that the 2-cluster to same 2-cluster S-matrix is a (non-classical, if the potentials are long-range) pseudo-differential operator which differs from the identity operator by an operator of order

-1. In our geometric normalization this means that they are Fourier integral operators associated to the geodesic flow on the sphere at infinity to distance π (along the cluster).

We remark that the results of these notes would remain valid if we assumed only that $V_a \in S^{-\rho}(X^a)$, $\rho > 0$, as customary. In fact, the proof of the propagation of singularities for generalized eigenfunctions remains essentially unchanged, and the only difference in the above Theorem is that the parametrix for the Poisson operators is not as explicit, cf. [31, 30]; instead, one needs to use the constructions of Isozaki-Kitada [15] (as presented by Skibsted and Bommier) directly. The reason for the polyhomogeneous assumption is that the proofs are somewhat nicer, especially in notation, and it is a particularly natural assumption to make in the compactification approach we adopt.

Our main tool in proving the propagation of singularities results consists of microlocally positive commutator estimates, i.e. on the construction of operators which have a positive commutator with H in the part of phase space, say U, where we wish to conclude that a generalized eigenfunction u has no scattering wave front set. These commutators are usually negative in another region of phase space, namely backwards (or forwards, depending on the construction) along generalized broken bicharacteristics through U. We thus assume the absence of this region from $\mathrm{WF}_{\mathrm{Sc}}(u)$, and conclude that the positive commutator region, U, is also missing from $\mathrm{WF}_{\mathrm{Sc}}(u)$. Such techniques have been used by Hörmander, Melrose and Sjöstrand [10, 20] to show the propagation of singularities for hyperbolic equations (real principal type propagation) such as the wave equation, including in regions with smooth boundaries. Indeed, the best way to interpret our results is to say that $H - \lambda$ is hyperbolic at infinity. In two-body scattering the analogy with the wave equation in domains without boundary is rather complete; this was the basis of Melrose's proof of propagation estimates for scattering theory for 'scattering metrics' in [19]. In many-body scattering, the lack of commutativity of the appropriate pseudo-differential algebra, even to top order, makes the estimates (and their proofs) more delicate. We remark that, as can be seen directly from the approach we take, the wave front set estimates can be easily turned into microlocal estimates on the resolvent considered as an operator between weighted Sobolev spaces; wave front set statements are a particularly convenient way of describing propagation.

Positive commutator estimates have also played a major role in many-body scattering starting with the work of Mourre [22], Perry, Sigal and Simon [23], Froese and Herbst [5], Jensen [16], Gérard, Isozaki and Skibsted [6, 7] and Wang [34]. 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 [13, 14, 32] in more detail.

More delicate (and often time-dependent) commutator estimates have been used in the 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 [24, 25, 27, 26, 8, 2, 35]. In particular, Yafaev's paper [35] shows quite explicitly the importance of the special structure of the Euclidean Hamiltonian. This structure enables him to obtain a (time-independent) positive commutator estimate, which would not follow from the indicial operator arguments of [33, 31, 30], and which is then used to prove asymptotic completeness.

We briefly mention the main idea, as presented in Froese's and Herbst's proof of the Mourre estimate [5], in showing that the commutator of $i\psi(H)A\psi(H)$ with H is positive, and in particular point out the role played by bound states. Here A is a certain self-adjoint operator, and $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$ is used to localize near the energy λ, so it is identically 1 near λ, supported sufficiently close to it. Thus, one shows (e.g. by a principal symbol calculation) that $i[\psi(H)A\psi(H), H] \geq C\psi(H)^2 + K$ where $C > 0$, and K is compact. Multiplying through by $\psi_1(H)$ from both sides, where ψ_1 is such that $\psi \equiv 1$ on $\operatorname{supp}\psi_1$, gives a similar estimate with ψ replaced by ψ_1, and K replaced by $\psi_1(H)K\psi_1(H)$. But if $\lambda \notin \operatorname{spec}_{pp}(H)$, then $\psi_1(H) \to 0$ strongly as $\operatorname{supp}\psi_1 \to \{\lambda\}$, so as K is compact, $\|\psi_1(H)K\psi_1(H)\| \to 0$ as $\operatorname{supp}\psi_1 \to \{\lambda\}$. Given any $\epsilon > 0$, we can thus arrange that $\psi_1(H)K\psi_1(H) \geq -\epsilon$. Substituting this into our inequality and multiplying it through by $\psi_2(H)$ from both sides, where ψ_2 is such that $\psi_1 \equiv 1$ on $\operatorname{supp}\psi_2$, gives $i[\psi_2(H)A\psi_2(H), H] \geq (C-\epsilon)\psi_2(H)^2$, i.e. eliminates the compact error term if ψ_2 has sufficiently small support near λ. Froese and Herbst use an inductive argument, starting at the free cluster, where a positivity estimate is trivial, to prove the Mourre estimate. In our setting, we perform such estimates for the indicial operators of a commutator, again starting at the free cluster. In the presence of bound states, the positivity will not come simply from such an argument; instead, one must have a positive commutator in the tangential (i.e. external) variables of the cluster to which the bound state is associated, positive when localized to the bound states (via the spectral projection of H).

These notes mostly consist of a summary of the results of [30], also reviewing some of the results of [31].

I am very grateful to Richard Melrose and Maciej Zworski for numerous very fruitful discussions; in particular, I would like to thank Richard Melrose for his comments on these lecture notes. I am grateful to Maciej Zworski for introducing me to the work of Gilles Lebeau [17]. If there are no bound states in any subsystems, many-body scattering is philosophically and, to a certain extent, technically (e.g. the structure of generalized broken bicharacteristics) is very similar to the wave equation in domain with corners. Thus, Lebeau's paper played an important direct role in my paper [31], and remained philosophically important while working on the present manuscript. I would also like to thank Andrew Hassell, Rafe Mazzeo, Erik Skibsted and Jared Wunsch for helpful discussions, their encouragement and for their interest in this research.

2. Notation and detailed statement of results

Before we can state the precise definitions, we need to introduce some basic (and mostly standard) notation. We refer to [3] for a very detailed discussion of the setup and the basic results. We consider the Euclidean space $\mathbb{R}^n$, and let g be the standard Euclidean metric on it. We assume also 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. We write g_a and g^a for the induced metrics on X_a and X^a respectively. We 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

$$H = \Delta + \sum_{a \in I} (\pi^a)^* V_a; \tag{2.1}$$

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:

$$V_a \in S^{-1}_{\text{phg}}(X^a). \tag{2.2}$$

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, here we use the conventional ordering, we simply write $X_a \subset X_b$ if the opposite ordering is required.) 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.

Our goal is to study generalized eigenfunctions of H, i.e. solutions $u \in \mathcal{S}'(\mathbb{R}^n)$ of $(H - \lambda)u = 0$. Since $H - \lambda$ is an elliptic partial differential operator with smooth coefficients, $(H - \lambda)u \in \mathcal{C}^\infty(\mathbb{R}^n)$ implies that $u \in \mathcal{C}^\infty(\mathbb{R}^n)$. Thus, the place where such u can have interesting behavior is at infinity. Analysis at infinity can be viewed either as analysis of uniform properties, or as that of properties in the appropriate compactification of $\mathbb{R}^n$. We adopt the second point of view by compactifying $\mathbb{R}^n$ as in [19]. Thus, we let $X = \mathbb{S}^n_+$ to be the radial compactification of $\mathbb{R}^n$ (also called the geodesic compactification) to a closed hemisphere, i.e. a ball, and $\mathbb{S}^{n-1} = \partial \mathbb{S}^n_+$. Recall from [19] that $\text{RC} : \mathbb{R}^n \to \mathbb{S}^n_+$ is given by

$$\text{RC}(w) = (1/(1 + |w|^2)^{1/2}, w/(1 + |w|^2)^{1/2}) \in \mathbb{S}^n_+ \subset \mathbb{R}^{n+1}, \quad w \in \mathbb{R}^n. \tag{2.3}$$

Here we use the notation RC instead of SP, used in [19], to avoid confusion with the standard stereographic projection giving a one-point compactification of $\mathbb{R}^n$. We write the coordinates on $\mathbb{R}^n = X_a \oplus X^a$ as (w_a, w^a). We let

$$\bar{X}_a = \text{cl}(\text{RC}(X_a)), \quad C_a = \bar{X}_a \cap \partial \mathbb{S}^n_+. \tag{2.4}$$

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

$$\mathcal{C} = \{C_a : \ a \in I\}. \tag{2.5}$$

Thus, $\bar{X}_0 = \mathbb{S}^n_+ = X$, $C_0 = \partial \mathbb{S}^n_+ = \mathbb{S}^{n-1}$, and $a \leq b$ if and only if $C_b \subset C_a$.

We note that if a is a 2-cluster then $C_a \cap C_b = \emptyset$ unless $C_a \subset C_b$, i.e. $b \leq a$. We also define the 'singular part' of C_a as the set

$$C_{a,\text{sing}} = \cup_{b \not\leq a} (C_b \cap C_a), \tag{2.6}$$

and its 'regular part' as the set

$$C'_a = C_a \setminus \cup_{b \not\leq a} C_b = C_a \setminus C_{a,\mathrm{sing}}. \tag{2.7}$$

For example, if a is a 2-cluster then $C_{a,\mathrm{sing}} = \emptyset$ and $C'_a = C_a$.

We usually identify (the interior of) $\mathbb{S}^n_+$ with $\mathbb{R}^n$. A particularly useful boundary defining function of $\mathbb{S}^n_+$ is given by $x \in \mathcal{C}^\infty(\mathbb{S}^n_+)$ defined as $x = r^{-1} = |w|^{-1}$ (for $r \geq 1$, say, smoothed out near the origin); so $\mathbb{S}^{n-1} = \partial\mathbb{S}^n_+$ is given by $x = 0$, $x > 0$ elsewhere, and $dx \neq 0$ at $\mathbb{S}^{n-1}$. We write $S^m_{\mathrm{phg}}(\mathbb{S}^n_+)$ and $S^m_{\mathrm{phg}}(\mathbb{R}^n)$ interchangeably. We also remark that

$$S^m_{\mathrm{phg}}(\mathbb{S}^n_+) = x^{-m}\mathcal{C}^\infty(\mathbb{S}^n_+). \tag{2.8}$$

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

$$H^{k,l}_{\mathrm{sc}}(\mathbb{S}^n_+) = H^{k,l} = H^{k,l}(\mathbb{R}^n) = \langle w\rangle^{-l} H^k(\mathbb{R}^n) \tag{2.9}$$

where $\langle w\rangle = (1 + |w|^2)^{1/2}$.

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

$$H^a = \Delta + \sum_{b \leq a} V_b, \tag{2.10}$$

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 (also called bound states) play an important role in many-body scattering; we remark that by a result of Froese and Herbst, [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

$$\Lambda_a = \cup_{b<a} \mathrm{spec}_{pp}(H^b) \tag{2.11}$$

be the set of thresholds of H^a, and we also let

$$\Lambda'_a = \Lambda_a \cup \mathrm{spec}_{pp}(H^a) = \cup_{b \leq a} \mathrm{spec}_{pp}(H^b). \tag{2.12}$$

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, 23]) 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

$$R(\lambda \pm i0) : H^{k,l}_{\mathrm{sc}}(\mathbb{S}^n_+) \to H^{k+2,l'}_{\mathrm{sc}}(\mathbb{S}^n_+) \tag{2.13}$$

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

$$\Lambda = \Lambda_1 \cup \mathrm{spec}_{pp}(H). \tag{2.14}$$

In addition, L^2 eigenfunctions of H^a with eigenvalues which are not thresholds are necessarily Schwartz functions on X^a (in fact, they decay exponentially, 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 phase space in scattering theory is the cotangent bundle $T^*\mathbb{R}^n$. Again, it is convenient to consider its appropriate partial compactification, i.e. to consider it as a vector bundle over $\mathbb{S}^n_+$. Thus, consider the set of all one-forms on $\mathbb{R}^n$ of the form

$$\sum_{j=1}^n a_j\,dw_j \tag{2.15}$$

where $a_j \in \mathcal{C}^\infty(\mathbb{S}^n_+)$ (we drop RC from the notation as usual). This is then the set of all smooth sections of a trivial vector bundle over $\mathbb{S}^n_+$, with basis $dw_1, \dots, dw_n$. Following Melrose's geometric approach to scattering theory, see [19], we consider this as the (dual) structure bundle, and call it the scattering cotangent bundle of $\mathbb{S}^n_+$, denoted by ${}^{\mathrm{sc}}T^*\mathbb{S}^n_+$. Note that $T^*\mathbb{R}^n$ can be identified with $\mathbb{R}^n\times\mathbb{R}^n$ via the metric g; correspondingly ${}^{\mathrm{sc}}T^*\mathbb{S}^n_+$ is identified with $\mathbb{S}^n_+\times\mathbb{R}^n$, i.e. we simply compactified the base of the standard cotangent bundle. We remark that the construction of ${}^{\mathrm{sc}}T^*\mathbb{S}^n_+$ is completely natural and geometric, just like the following ones, see [19], or Section 3 for a summary.

However, in many-body scattering ${}^{\mathrm{sc}}T^*\mathbb{S}^n_+$ is *not* the natural place for microlocal analysis for the very same reason that introduces the compressed cotangent bundle in the study of the wave equation on bounded domains. We can see what causes trouble from both the dynamical and the quantum point of view. Regarding dynamics, the issue is that only the external part of the momentum is preserved in a collision, the internal part is not; while from the quantum point of view the problem is that there is only partial commutativity in the algebra of the associated pseudo-differential operators, even to top order. To rectify this, we replace the full bundle ${}^{\mathrm{sc}}T^*_{C'_a}\mathbb{S}^n_+ = C'_a\times\mathbb{R}^n$ over $C'_a\subset\mathbb{S}^{n-1}$ by ${}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a = C'_a\times X_a$, i.e. we consider

$${}^{\mathrm{sc}}\dot{T}^*\mathbb{S}^n_+ = \cup_a\,{}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a. \tag{2.16}$$

Over C'_a, there is a natural projection $\pi_a : {}^{\mathrm{sc}}T^*_{C'_a}\mathbb{S}^n_+ \to {}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a$ corresponding to the pull-back of one-forms; in the trivialization given by the metric it is induced by the orthogonal projection to X_a in the fibers. By putting the π_a together, we obtain a projection $\pi : {}^{\mathrm{sc}}T^*_{\mathbb{S}^{n-1}}\mathbb{S}^n_+ \to {}^{\mathrm{sc}}\dot{T}^*\mathbb{S}^n_+$. We put the topology induced by π on ${}^{\mathrm{sc}}\dot{T}^*\mathbb{S}^n_+$. This definition is analogous to that of the compressed cotangent bundle in the works of Melrose, Sjöstrand [20] and Lebeau [17] on the wave equation in domains with smooth boundaries or corners, respectively.

We also recall from [19] that the characteristic variety $\Sigma_0(\lambda)$ of $\Delta-\lambda$ is simply the subset of ${}^{\mathrm{sc}}T^*_{\mathbb{S}^{n-1}}\mathbb{S}^n_+$ where $g-\lambda$ vanishes; g being the metric function. If $\Lambda_1=\{0\}$, the compressed characteristic set of $H-\lambda$ will be simply $\pi(\Sigma_0(\lambda))\subset{}^{\mathrm{sc}}\dot{T}^*\mathbb{S}^n_+$. In general, all the bound states contribute to the characteristic variety. Thus, we let

$$\Sigma_b(\lambda) = \{\xi_b \in {}^{\mathrm{sc}}T^*_{C_b}\bar{X}_b :\ \lambda - |\xi_b|^2 \in \operatorname{spec}_{pp} H^b\} \subset {}^{\mathrm{sc}}T^*_{C_b}\bar{X}_b; \tag{2.17}$$

note that $|\xi_b|^2$ is the kinetic energy of a particle in a bound state of H^b. If $C_a\subset C_b$, there is also a natural projection $\pi_{ba} : {}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_b \to {}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a$ (in the metric trivialization we can use the orthogonal projection $X_b\to X_a$ as above), and then we define the characteristic set of $H-\lambda$ to be

$$\dot{\Sigma}(\lambda) = \cup_a\dot{\Sigma}_a(\lambda), \qquad \dot{\Sigma}_a(\lambda) = \cup_{C_b\supset C_a}\pi_{ba}(\Sigma_b(\lambda))\cap{}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a, \tag{2.18}$$

so $\dot{\Sigma}(\lambda)\subset{}^{\mathrm{sc}}\dot{T}^*\mathbb{S}^n_+$. We let $\hat{\pi}_b$ be the restriction of $\pi_b : {}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_b \to \dot{\Sigma}(\lambda)$ to $\Sigma_b(\lambda)$.

We next recall from [31] the definition of generalized broken bicharacteristics in case there are no bound states in any of the subsystems. In fact, in this case the word 'generalized' can be dropped; for the generalized broken bicharacteristics have a simple geometry as stated below. First, note that the rescaled Hamilton vector field of the metric function g, i.e.

$$2\langle w\rangle\xi\cdot\partial_w\in\mathcal{V}(T^*\mathbb{R}^n)=\mathcal{V}(\mathbb{R}^n\times\mathbb{R}^n) \tag{2.19}$$

extends to a smooth vector field, ${}^{\mathrm{sc}}H_g\in\mathcal{V}({}^{\mathrm{sc}}T^*\mathbb{S}^n_+)=\mathcal{V}(\mathbb{S}^n_+\times\mathbb{R}^n)$, with $\mathbb{S}^n_+$ considered as the radial compactification of $\mathbb{R}^n$; in fact, ${}^{\mathrm{sc}}H_g$ is tangent to the boundary ${}^{\mathrm{sc}}T^*_{\mathbb{S}^{n-1}}\mathbb{S}^n_+=\mathbb{S}^{n-1}\times\mathbb{R}^n$.

Definition. Suppose $\Lambda_1=\{0\}$, and $I=[\alpha,\beta]$ is an interval. We say that a continuous map $\gamma:I\to\dot\Sigma(\lambda)$ is a broken bicharacteristic of $H-\lambda$ if 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 the image of an integral curve of ${}^{\mathrm{sc}}H_g$ in $\Sigma_0(\lambda)$ under π. If I is an interval (possibly $\mathbb{R}$), we say that $\gamma:I\to\dot\Sigma(\lambda)$ is a broken bicharacteristic of $H-\lambda$, if the restriction of γ to every compact subinterval of I is a broken bicharacteristic in the above sense.

Here $\gamma(I)\subset\dot\Sigma(\lambda)=\pi(\Sigma_0(\lambda))$ corresponds to the conservation of kinetic energy in collisions (since there are no bound states), and the use of the compressed space ${}^{\mathrm{sc}}\dot T^*\mathbb{S}^n_+$ shows that external momentum is conserved in the collisions. It turns out, see [31], that γ is essentially the lift of a broken geodesic on $\mathbb{S}^n_+$ of length π (if $I=\mathbb{R}$, otherwise shorter), broken at the collision planes, i.e. at $\mathcal{C}$. In particular, even if $I=\mathbb{R}$, it has only a finite number of breaks, and in fact, there is a uniform bound on the number of such breaks (depending only on the geometry, i.e. on $\mathcal{C}$, not on γ).

The definitions are less explicit if $\Lambda_1\neq\{0\}$, but they essentially still state that the total energy and the external momentum are preserved in collisions. Thus, generalized broken bicharacteristics will be continuous maps γ defined on intervals I, $\gamma:I\to\dot\Sigma(\lambda)$ with certain appropriate generalization of the integral curve condition described above. In order to take the bound states into consideration, we also need to consider the rescaled Hamilton vector fields ${}^{\mathrm{sc}}H^b_g$ of the metric g_b in the subsystem b. Thus, under the inclusion map

$$\imath_b:{}^{\mathrm{sc}}T^*_{C_b}\bar X_b\hookrightarrow{}^{\mathrm{sc}}T^*_{C_b}\mathbb{S}^n_+ \tag{2.20}$$

induced by the inclusion $X_b\hookrightarrow\mathbb{R}^n$ in the fibers, $(\imath_b)_*{}^{\mathrm{sc}}H^b_g={}^{\mathrm{sc}}H_g$ (i.e. the restriction of the vector field ${}^{\mathrm{sc}}H_g$ to ${}^{\mathrm{sc}}T^*_{C_b}\bar X_b$, considered as a subset of ${}^{\mathrm{sc}}T^*_{C_b}\mathbb{S}^n_+$). Thus, we require that lower bounds on the Hamilton vector fields ${}^{\mathrm{sc}}H^b_g$ applied to π-invariant functions, i.e. to functions $f\in\mathcal{C}^\infty({}^{\mathrm{sc}}T^*_{\mathbb{S}^{n-1}}\mathbb{S}^n_+)$ such that $f(\xi)=f(\xi')$ if $\pi(\xi)=\pi(\xi')$, imply lower bounds on the derivatives of f_π along γ. Here f_π is the function induced by f on ${}^{\mathrm{sc}}\dot T^*\mathbb{S}^n_+$, so $f=f_\pi\circ\pi$.

Definition 2.1. A generalized broken bicharacteristic of $H-\lambda$ is a continuous map $\gamma:I\to\dot\Sigma(\lambda)$, where $I\subset\mathbb{R}$ is an interval, such that for all $t_0\in I$ and for each sign $+$ and $-$ the following holds. Let $\xi_0=\gamma(t_0)$, suppose that $\xi_0\in{}^{\mathrm{sc}}T^*_{C'_a}\bar X_a$. Then for all π-invariant functions $f\in\mathcal{C}^\infty({}^{\mathrm{sc}}T^*_{\mathbb{S}^{n-1}}\mathbb{S}^n_+)$,

$$D_\pm(f_\pi\circ\gamma)(t_0)\geq\inf\{{}^{\mathrm{sc}}H^b_gf(\tilde\xi_0):\ \tilde\xi_0\in\hat\pi_b^{-1}(\xi_0),\ C_a\subset C_b\}. \tag{2.21}$$

Here $D_\pm$ are the one-sided lower derivatives: if g is defined on an interval I, $(D_\pm g)(t_0)=\liminf_{t\to t_0\pm}(g(t)-g(t_0))/(t-t_0)$.

Although it is not apparent, this definition is equivalent to the previous one if $\Lambda_1 = \{0\}$. Moreover, in four-body scattering, even if $\Lambda_1 \neq \{0\}$, one can describe the generalized broken bicharacteristics piecewise as projections of integral curves of ${}^{\mathrm{sc}}H_g$. In general many-body scattering, the lack of conservation of kinetic energy makes such a description harder, but if Λ_1 is discrete, we obtain a description that parallels the one above. More precisely, suppose that Λ_1 is discrete and $\gamma : \mathbb{R} \to \dot{\Sigma}(\lambda)$ is a continuous curve. Then γ is a generalized broken bicharacteristic of $H - \lambda$ if and only if there exist $t_0 < t_1 < t_2 < \ldots < t_k$ such that $\gamma|_{[t_j, t_{j+1}]}$, as well as $\gamma|_{(-\infty, t_0]}$ and $\gamma|_{[t_k, +\infty)}$, are the projections of integral curves of the Hamilton vector field ${}^{\mathrm{sc}}H_g^a$ for some a. In addition, there is a uniform bound on k (independent of γ), depending only on $\mathcal{C}$ and Λ_1. Similar results hold if the interval of definition, $\mathbb{R}$, is replaced by any interval.

As mentioned in the introduction, 'singularities' (i.e. lack of decay at infinity) of $u \in \mathcal{S}'$ are described by the many-body scattering wave front set, $\mathrm{WF}_{\mathrm{Sc}}(u)$, which was introduced in [31], and which describes u modulo Schwartz functions, similarly to how the usual wave front set describes distributions modulo smooth functions. Just as for the image of the bicharacteristics, ${}^{\mathrm{sc}}\dot{T}^*\mathbb{S}^n_+$ provides the natural setting in which $\mathrm{WF}_{\mathrm{Sc}}$ is defined: $\mathrm{WF}_{\mathrm{Sc}}(u)$ is a closed subset of ${}^{\mathrm{sc}}\dot{T}^*\mathbb{S}^n_+$. The definition of $\mathrm{WF}_{\mathrm{Sc}}(u)$ relies on the algebra of many-body scattering pseudo-differential operators, also introduced in [31].

Here we will not define these; rather we will translate our results into statements on the S-matrices where the usual wave front set can be used. However, at the end of these notes we give a short discussion of the required constructions. In addition, in the two-body setting, when ${}^{\mathrm{sc}}\dot{T}^*\mathbb{S}^n_+ = {}^{\mathrm{sc}}T^*\mathbb{S}^n_+$, $\mathrm{WF}_{\mathrm{Sc}}$ is just the scattering wave front set $\mathrm{WF}_{\mathrm{sc}}$ introduced by Melrose, [19], which in turn is closely related to the usual wave front set via the Fourier transform. Thus, for $(\omega, \xi) \in {}^{\mathrm{sc}}T^*_{\mathbb{S}^{n-1}}\mathbb{S}^n_+$, considered as $\mathbb{S}^{n-1} \times \mathbb{R}^n = \partial\mathbb{S}^n_+ \times \mathbb{R}^n$, $(\omega, \xi) \notin \mathrm{WF}_{\mathrm{sc}}(u)$ means that there exists $\phi \in \mathcal{C}^\infty(\mathbb{S}^n_+)$ such that $\phi(\omega) \neq 0$ and $\mathcal{F}(\phi u)$ is $\mathcal{C}^\infty$ near ξ. If we employed the usual conic terminology instead of the compactified one, we would think of ϕ as a conic cut-off function in the direction ω. Thus, $\mathrm{WF}_{\mathrm{sc}}$ at infinity is analogous to WF with the role of position and momentum reversed. We also remark that we state all of the following results for the absolute wave front sets (i.e. we work modulo Schwartz functions), but they have complete analogues for the relative wave front sets (working modulo weighted Sobolev spaces); indeed, it is the latter that is used to prove the results on the former.

Our main result is then the following theorem, in which we allow arbitrary thresholds, and which describes the relationship between $\mathrm{WF}_{\mathrm{Sc}}(u)$ and generalized broken bicharacteristics, if, for example, $(H - \lambda)u = 0$.

Theorem 2.2. *Let $u \in \mathcal{S}'(\mathbb{R}^n)$, $\lambda \notin \Lambda_1$. Then*

$$\mathrm{WF}_{Sc}(u) \setminus \mathrm{WF}_{Sc}((H - \lambda)u) \tag{2.22}$$

is a union of maximally extended generalized broken bicharacteristics of $H - \lambda$ in $\dot{\Sigma}(\lambda) \setminus \mathrm{WF}_{Sc}((H - \lambda)u)$.

We remark that the statement of the theorem is empty at points $\xi_0 \in {}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a$ at which ${}^{\mathrm{sc}}H_g^b(\tilde{\xi}_0) = 0$ for some $\tilde{\xi}_0 \in \hat{\pi}_b^{-1}(\xi_0)$ and some b with $C_a \subset C_b$. Indeed, at such points the constant curve ($\gamma(t) = \tilde{\xi}_0$ for all t in some interval) is a generalized broken bicharacteristic. A simple calculation shows that the set of these points ξ_0

is $R_+(\lambda)\cup R_-(\lambda)$, where

(2.23)

$$R_\pm(\lambda)=\{\xi\in {}^{\mathrm{sc}}T^*_{C'_a}\bar X_a:\ \exists b,\ C_a\subset C_b, \lambda-\tau(\xi)^2\in\mathrm{spec}_{pp}(H^b),\ \pm\tau(\xi)\geq 0\}$$

are the incoming $(+)$ and outgoing $(-)$ radial sets respectively, and τ is the sc-dual variable of the boundary defining function x, so in terms of the Euclidean variables

$$\tau=-\frac{w\cdot\xi}{|w|}; \tag{2.24}$$

see the next section for further details. Hence, the theorem permits singularities to emerge 'out of nowhere' at the radial sets. Although we do not prove that this indeed does happen, based on general principles, this appears fairly likely. Moreover, the optimality of Theorem 2.2 if $\Lambda_1=\{0\}$ follows from [9, 29], see the remarks about this in [31]; the amplitude of the reflected 'wave' is given (to top order) by the appropriate subsystem S-matrix.

There is a similar result for $\mathrm{WF}_{\mathrm{Sc}}(u)$, $u=R(\lambda+i0)f$; namely that $\mathrm{WF}_{\mathrm{Sc}}(u)\setminus\mathrm{WF}_{\mathrm{Sc}}(f)$ is the image of $\mathrm{WF}_{\mathrm{Sc}}(f)\cup R_-(\lambda)$ under forward propagation, if e.g. $f\in H^{r,s}$, $s>1/2$. The set $R_-(\lambda)$ appears here since there can be maximally extended generalized broken bicharacteristics which are either not disjoint from $R_-(\lambda)$, or simply whose closure is not disjoint from $R_-(\lambda)$. In particular, even if f is Schwartz, $\mathrm{WF}_{\mathrm{Sc}}(u)$ is not necessarily a subset of $R_-(\lambda)$, rather a subset of its image under forward propagation. Indeed, by duality, this is exactly what gives rise to the conditions on $\mathrm{WF}_{\mathrm{Sc}}(f)$ under which $u=R(\lambda+i0)f$ can be defined. To make it easier to state these results, we make the following definition.

Definition 2.3. Suppose $K\subset\dot\Sigma(\lambda)$. The image $\Phi_+(K)$ of K under the forward broken bicharacteristic relation is defined as

(2.25)

$$\begin{aligned}\Phi_+(K)=\{&\xi_0\in\dot\Sigma(\lambda):\ \exists\text{ a generalized broken bicharacteristic }\gamma:(-\infty,t_0]\to\dot\Sigma(\lambda)\\ &\text{s.t. }\gamma(t_0)=\xi_0,\ \overline{\gamma((-\infty,t_0])}\cap K\neq\emptyset\}.\end{aligned}$$

The image $\Phi_-(K)$ of K under the backward broken bicharacteristic relation is defined similarly, with $[t_0,+\infty)$ in place of $(-\infty,t_0]$.

Note that $\Phi_+(K)=\cup_{\xi\in K}\Phi_+(\{\xi\})$ directly from the definition. The result on the boundary values of the resolvent is then:

Theorem 2.4. *Suppose that $\lambda\notin\Lambda$, $f\in\mathcal{S}(\mathbb{R}^n)$, and let $u=R(\lambda+i0)f$. Then $\mathrm{WF}_{Sc}(u)\subset\Phi_+(R_-(\lambda))$. Moreover, $R(\lambda+i0)$ extends by continuity to $v\in\mathcal{S}'(\mathbb{R}^n)$ with $\mathrm{WF}_{Sc}(v)\cap\Phi_-(R_+(\lambda))=\emptyset$, and for such v,*

$$\mathrm{WF}_{Sc}(R(\lambda+i0)v)\subset\Phi_+(\mathrm{WF}_{Sc}(v))\cup\Phi_+(R_-(\lambda)). \tag{2.26}$$

The scattering matrices $S_{\beta\alpha}(\lambda)$ of H with incoming channel α, outgoing channel β can be defined either via the wave operators, or via the asymptotic behavior of generalized eigenfunctions. It was shown in [32] that the two are the same, up to normalization (free motion is factored out in the wave operator definition); here we briefly recall the second definition. We first state it for short-range V_c (V_c polyhomogeneous of order -2 for all c). Thus, for $\lambda\in(\epsilon_\alpha,\infty)\setminus\Lambda$ and $g\in\mathcal{C}^\infty_c(C'_a)$, there is a unique $u\in\mathcal{S}'(\mathbb{R}^n)$ such that $(H-\lambda)u=0$, and u has the form

$$u=e^{-i\sqrt{\lambda-\epsilon_\alpha}r}r^{-\dim C_a/2}((\pi^a)^*\psi_\alpha)v_-+R(\lambda+i0)f, \tag{2.27}$$

where $v_- \in \mathcal{C}^\infty(\mathbb{S}^n_+)$, $v_-|_{C_a} = g$, and $f \in H^{\infty,1/2+\epsilon'}_{\mathrm{sc}}(\mathbb{S}^n_+)$, $\epsilon' > 0$. The Poisson operator $P_{\alpha,+}(\lambda)$ is the map

$$P_{\alpha,+}(\lambda) : \mathcal{C}^\infty_c(C'_a) \to \mathcal{S}'(\mathbb{R}^n) \text{ defined by } P_{\alpha,+}(\lambda)g = u. \tag{2.28}$$

The term $R(\lambda + i0)$ has distributional asymptotics of a similar form 'at the channel β', i.e. of the form $e^{i\sqrt{\lambda-\epsilon_\beta}r} r^{-\dim C_b/2}((\pi^b)^*\psi_\beta)v_{\beta,+}$, see [32] for the precise definitions.

Only minor modifications are necessary for $V_c \in S^{-1}_{\mathrm{phg}}(X^c)$. Namely, write

$$I_a = \sum_{b \not\leq a} V_b,\ \tilde{I}_a = (r_a I_a)|_{C_a} \in \mathcal{C}^\infty(C_a), \tag{2.29}$$

I_a is $\mathcal{C}^\infty$ near C'_a with simple vanishing at C'_a (since $b \not\leq a$ means $C_a \not\subset C_b$, hence $C_a \cap C_b \subset C_{a,\mathrm{sing}}$), so $r_a I_a$ is $\mathcal{C}^\infty$ there. Then the asymptotics in (2.27) must be replaced by

$$e^{-i\sqrt{\lambda-\epsilon_\beta}r} r^{-\dim C_a/2} r^{i\tilde{I}_a/2\sqrt{\lambda-\epsilon_\alpha}}((\pi^a)^*\psi_\alpha)v_-. \tag{2.30}$$

The scattering matrix $S_{\beta\alpha}(\lambda)$ maps $g = v_-|_{C_a}$ to $v_{\beta,+}|_{C'_b}$. It is also given by the formula

$$S_{\beta\alpha}(\lambda) = \frac{1}{2i\sqrt{\lambda-\epsilon_\beta}}((H-\lambda)\tilde{P}_{\beta,-}(\lambda))^* P_{\alpha,+}(\lambda), \tag{2.31}$$

$\lambda > \max(\epsilon_\alpha, \epsilon_\beta)$, $\lambda \notin \Lambda$. Here $\tilde{P}_{\beta,-}(\lambda)$ is a microlocalized version of the outgoing Poisson operator, microlocalized near the outgoing region for β, i.e. where τ is near $-\sqrt{\lambda-\epsilon_\beta}$, see [32]. In fact, we can simply take $\tilde{P}_{\beta,-}(\lambda)$ to be a microlocal (cut-off) parametrix for $P_{\beta,-}(\lambda)$. This formula is closely related to that of Isozaki and Kitada [15].

A very good parametrix, $\tilde{P}_{\alpha,+}(\lambda)$, for $P_{\alpha,+}(\lambda)$ in the region of phase space where τ is close to $\sqrt{\lambda-\epsilon_\alpha}$ has been constructed by Skibsted [28] in the short-range and by Bommier [1] in the long-range setting, under the assumption that $\epsilon_\alpha \in \mathrm{spec}_d(H^a)$. If we instead assume that the V_c are all Schwartz, then the trivial (product type) construction gives the desired parametrix. Their constructions enable us to deduce the structure of the S-matrices immediately from our propagation theorem, Theorem 2.4 via (2.31) and

$$P_{\alpha,+}(\lambda) = \tilde{P}_{\alpha,+}(\lambda) - R(\lambda + i0)(H-\lambda)\tilde{P}_{\alpha,+}(\lambda). \tag{2.32}$$

Since the parametrix (near the incoming or outgoing sets) is important for turning the results on the propagation of singularities to wave front set results, in all our results on the Poisson operators and S-matrices $S_{\beta\alpha}(\lambda)$ in these notes we make the following assumption:

$$\text{either } \epsilon_\alpha \in \mathrm{spec}_d(H^a) \text{ and } \epsilon_\beta \in \mathrm{spec}_d(H^b), \text{ or } V_c \in \mathcal{S}(X^c) \text{ for all } c. \tag{2.33}$$

It is easy to describe the wave front set of $\tilde{P}_{\alpha,+}(\lambda)g$, $g \in \mathcal{C}^{-\infty}_c(C'_a)$, near its 'beginning point', i.e. near the $(\alpha,+)$-incoming set. Namely, it is the union of integral curves of ${}^{\mathrm{sc}}H^a_g$ (in ${}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a$) (which are in particular bicharacteristics of $H-\lambda$, hence broken bicharacteristics), one integral curve for each $\zeta \in \mathrm{WF}(g) \subset S^*C'_a$; we denote these integral curves by $\gamma_{\alpha,-}(\zeta)$. It is actually convenient to replace the parameter t of the integral curve by s, the arclength parameter of its projection to C_a. The relationship between these two is that if we write $s = S(t)$, then S solves the ODE $dS/dt = 2(\lambda - \epsilon_\alpha - \tau(\gamma(t))^2)^{1/2}$. The reparameterized integral curves are then given by

(2.34)
$$\tau_a = \sqrt{\lambda - \epsilon_\alpha}\cos(s - s_0),\ (y_a, \mu_a) = \sqrt{\lambda - \epsilon_\alpha}\sin(s - s_0)\exp((s - s_0)^{\mathrm{sc}} H_g^a)(\zeta)$$

where $s \in (s_0, s_0 + \pi)$. This defines $\gamma_{\alpha,-}(\zeta)$ up to replacing t by $t - t_1$ for any fixed $t_1 \in \mathbb{R}$, so we are abusing the notation slightly. Due to (2.32), Theorem 2.4 describes $\mathrm{WF}_{\mathrm{Sc}}(P_{\alpha,+}(\lambda)g)$ elsewhere. A similar result also applies for $\tilde{P}_{\beta,-}(\lambda)$; in this case one simply has to replace the range of the arclength parameter by $s \in (s_0 - \pi, s_0)$. We denote the corresponding integral curves by $\gamma_{\beta,+}(\zeta)$.

Definition 2.5. The forward broken bicharacteristic relation with initial channel α is defined to be the relation $\mathcal{R}_{\alpha,+} \subset S^*C'_a \times \dot{\Sigma}(\lambda)$ given by

$$\mathcal{R}_{\alpha,+} = \{(\zeta, \xi) \in S^*C'_a \times \dot{\Sigma}(\lambda) :\ \Phi_-(\{\xi\}) \cap \gamma_{\alpha,-}(\zeta) \neq \emptyset\}. \tag{2.35}$$

The backward broken bicharacteristic relation with initial channel β, denoted by $\mathcal{R}_{\beta,-}$ is defined similarly, with Φ_+ in place of Φ_- and $\gamma_{\beta,+}$ in place of $\gamma_{\alpha,-}$. Finally, the forward broken bicharacteristic relation with initial channel α, final channel β, $\mathcal{R}_{\alpha\beta} \subset S^*C'_a \times S^*C'_b$ is defined as the composite relation of $\mathcal{R}_{\alpha,+}$ and $\mathcal{R}_{\beta,-}^{-1}$:

(2.36)
$$\mathcal{R}_{\alpha\beta} = \{(\zeta, \zeta') \in S^*C'_a \times S^*C'_b :\ \exists \xi \in \dot{\Sigma}(\lambda), (\zeta, \xi) \in \mathcal{R}_{\alpha,+},\ (\zeta', \xi) \in \mathcal{R}_{\beta,-}\}.$$

Note that $(\zeta, \xi) \in \mathcal{R}_{\alpha,+}$ thus means that there exists a generalized broken bicharacteristic $\gamma : \mathbb{R} \to \dot{\Sigma}(\lambda)$ and $t_0 \in \mathbb{R}$ such that $\gamma|_{(-\infty,t_0]}$ is given by $\gamma_{\alpha,-}(\zeta)$, and $\xi \in \overline{\gamma([t_0, +\infty))}$. Thus, $\mathcal{R}_{\alpha,+}$ should be thought of as the relation induced by Φ_- 'at channel α' as time goes to $-\infty$.

If $\mathcal{R} \subset A \times B$ is a relation, $K \subset A$, by $\mathcal{R}(K)$ we mean $\{\xi \in B :\ \exists \zeta \in K,\ (\zeta, \xi) \in \mathcal{R}\}$. Similarly, if $U \subset B$, by $\mathcal{R}^{-1}(U)$ we mean $\{\zeta \in A :\ \exists \xi \in U,\ (\zeta, \xi) \in \mathcal{R}\}$. We call $\mathcal{R}(K)$ the image of K under $\mathcal{R}$. Thus, if $K \subset S^*C'_a$,

$$\mathcal{R}_{\alpha,+}(K) = \{\xi \in \dot{\Sigma}(\lambda) :\ \exists \zeta \in K,\ \Phi_-(\{\xi\}) \cap \gamma_{\alpha,-}(\zeta) \neq \emptyset\},$$

and if $U \subset \dot{\Sigma}(\lambda)$, then

$$\mathcal{R}_{\alpha,+}^{-1}(U) = \{\zeta \in S^*C'_a :\ \exists \xi \in U,\ \Phi_-(\{\xi\}) \cap \gamma_{\alpha,-}(\zeta) \neq \emptyset\}.$$

This definition, (2.32) and Theorem 2.4 immediately prove the following proposition.

Proposition 2.6. *Suppose that H is a many-body Hamiltonian, $\lambda \notin \Lambda$, and (2.33) holds. Suppose also that $g \in \mathcal{C}_c^\infty(C'_a)$. Then*

$$\mathrm{WF}_{Sc}(P_{\alpha,+}(\lambda)g) \setminus R_+(\lambda) \subset \Phi_+(R_-(\lambda)). \tag{2.37}$$

In addition, $P_{\alpha,+}(\lambda)$ extends by continuity from $\mathcal{C}_c^\infty(C'_a)$ to distributions $g \in \mathcal{C}_c^{-\infty}(C'_a)$ with $(\mathrm{WF}(g) \times R_+(\lambda)) \cap \mathcal{R}_{\alpha,+} = \emptyset$ (i.e. $\mathcal{R}_{\alpha,+}(\mathrm{WF}(g)) \cap R_+(\lambda) = \emptyset$). If g is such a distribution, then

$$\mathrm{WF}_{Sc}(P_{\alpha,+}(\lambda)g) \subset \Phi_+(R_-(\lambda)) \cup \mathcal{R}_{\alpha,+}(\mathrm{WF}(g)). \tag{2.38}$$

One of the main features of (2.37) is that in general $\mathrm{WF}_{\mathrm{Sc}}(P_{\alpha,+}(\lambda)g)$ cannot be expected to be contained in the radial sets; one also has to include the image of the outgoing radial set under forward propagation in the statement. As a corollary, (2.31) shows that in general $S_{\beta\alpha}(\lambda)$ does not map smooth incoming data to smooth outgoing data. However, if β is a two-cluster channel, every generalized broken bicharacteristic γ such that for some $t_0 \in \mathbb{R}$, $\gamma|_{(-\infty,t_0]}$ is given by $\gamma_{\beta,+}(\zeta)$, $\zeta \in S^*C'_b$, is actually equal to $\gamma_{\beta,+}(\zeta)$ for all times, and, b being a 2-cluster, $\gamma_{\beta,+}(\zeta)$ never intersects the radial sets, and as $t \to \pm\infty$, $\gamma_{\beta,+}(\zeta)(t)$ goes to $R_{\mp}(\lambda)$. Thus, if β is a 2-cluster, α is any cluster, $S_{\beta\alpha}(\lambda)$ maps smooth functions to smooth functions. On the other hand, if β is the free channel 0, then the absence of positive thresholds gives a similar conclusion.

Corollary 2.7. *Suppose that H is a many-body Hamiltonian, $\lambda \notin \Lambda$, and (2.33) holds. Suppose $g \in \mathcal{C}_c^\infty(C'_a)$. Then $\mathrm{WF}(S_{\beta\alpha}(\lambda)g) \subset \mathcal{R}_{\beta,-}^{-1}(R_-(\lambda))$. Thus, if β is the free channel or it is a two-cluster channel, then $S_{\beta\alpha}(\lambda)g$ is $\mathcal{C}^\infty$.*

Our theorem on the wave front relation of the S-matrix is then the following.

Theorem 2.8. *Suppose that H is a many-body Hamiltonian, $\lambda \notin \Lambda$, and (2.33) holds. Then $S_{\beta\alpha}$ extends by continuity from $\mathcal{C}_c^\infty(C'_a)$ to distributions $g \in \mathcal{C}_c^{-\infty}(C'_a)$ with $\mathcal{R}_{\alpha,+}(\mathrm{WF}(g)) \cap R_+(\lambda) = \emptyset$. If g is such a distribution, then*

$$\mathrm{WF}_{Sc}(S_{\beta\alpha}(\lambda)g) \subset \mathcal{R}_{\beta,-}^{-1}(R_-(\lambda)) \cup \mathcal{R}_{\alpha\beta}(\mathrm{WF}(g)). \tag{2.39}$$

If $\Lambda_1 = \{0\}$, then maximally extended generalized broken bicharacteristics are essentially the lift of generalized broken geodesics on $\mathbb{S}^{n-1}$ of length π, so in this case we recover the following result of [31].

Corollary 2.9. *If no subsystem of H has bound states and $\lambda > 0$, then the wave front relation of $S_{00}(\lambda)$ is given by the broken geodesic relation on $\mathbb{S}^{n-1}$, broken at $\mathcal{C}$, at distance π.*

3. Scattering geometry and analysis

Although we cannot present a discussion of the required pseudo-differential constructions here, in this section we point out the main features of many-body scattering from the viewpoint of the compactification approach we adopted, using only the appropriate differential operator algebras.

First, we recall from [19] Melrose's definition of the Lie algebra of 'scattering vector fields' $\mathcal{V}_{\mathrm{sc}}(X)$, defined for every manifold with boundary X. Thus,

$$\mathcal{V}_{\mathrm{sc}}(X) = x\mathcal{V}_{\mathrm{b}}(X) \tag{3.1}$$

where $\mathcal{V}_{\mathrm{b}}(X)$ is the set of smooth vector fields on X which are tangent to ∂X. If $(x, y_1, \ldots, y_{n-1})$ are coordinates on X where x is a boundary defining function, then locally a basis of $\mathcal{V}_{\mathrm{sc}}(X)$ is given by

$$x^2\partial_x,\ x\partial_{y_j},\ j = 1, \ldots, n-1. \tag{3.2}$$

Correspondingly, there is a vector bundle ${}^{\mathrm{sc}}TX$ over X, called the scattering tangent bundle of X, such that $\mathcal{V}_{\mathrm{sc}}(X)$ is the set of all smooth sections of ${}^{\mathrm{sc}}TX$:

$$\mathcal{V}_{\mathrm{sc}}(X) = \mathcal{C}^\infty(X; {}^{\mathrm{sc}}TX). \tag{3.3}$$

The dual bundle of ${}^{\mathrm{sc}}TX$ (called the scattering cotangent bundle) is denoted by ${}^{\mathrm{sc}}T^*X$. Thus, covectors $v \in {}^{\mathrm{sc}}T^*_pX$, p near ∂X, can be written as

$$v = \tau\frac{dx}{x^2} + \mu \cdot \frac{dy}{x}. \tag{3.4}$$

Hence, we have local coordinates (x, y, τ, μ) on ${}^{\mathrm{sc}}T^*X$ near ∂X. Finally, $\mathrm{Diff}_{\mathrm{sc}}(X)$ is the algebra of differential operators generated by the vector fields in $\mathcal{V}_{\mathrm{sc}}(X)$; $\mathrm{Diff}^m_{\mathrm{sc}}(X)$ stands for scattering differential operators of order (at most) m.

An example is provided by the radial compactification of Euclidean space, $X = \mathbb{S}^n_+$. We can use 'inverse' polar coordinates on $\mathbb{R}^n$ to induce local coordinates on $\mathbb{S}^n_+$ near $\partial\mathbb{S}^n_+$ as above. Thus, we let $x = r^{-1} = |w|^{-1}$ (for $r \geq 1$, say, smoothed out near the origin), as in the introduction, write $w = x^{-1}\omega$, $\omega \in \mathbb{S}^{n-1}$, $|w| > 1$, and let y_j, $j = 1, \ldots, n-1$, be local coordinates on $\mathbb{S}^{n-1}$. For example, one can take the y_j to be $n-1$ of the $w_k/|w|$, $k = 1, \ldots, n$. Then $x \in \mathcal{C}^\infty(\mathbb{S}^n_+)$ is a boundary defining function of $\mathbb{S}^n_+$, and x and the y_j give local coordinates near $\partial\mathbb{S}^n_+ = \mathbb{S}^{n-1}$.

To establish the relationship between the scattering structure and the Euclidean scattering theory, we identify $\mathbb{S}^n_+$ with $\mathbb{R}^n$ via the radial compactification RC as in (2.3). The constant coefficent vector fields ∂_{w_j} on $\mathbb{R}^n$ lift under RC to give a basis of ${}^{\mathrm{sc}}T\mathbb{S}^n_+$. Thus, $P \in \mathrm{Diff}^m_{\mathrm{sc}}(\mathbb{S}^n_+)$ can be expressed as (ignoring the lifting in the notation)

$$P = \sum_{|\alpha| \leq m} a_\alpha \partial_w^\alpha, \quad a_\alpha \in \mathcal{C}^\infty(\mathbb{S}^n_+). \tag{3.5}$$

As mentioned above, $a_\alpha \in \mathcal{C}^\infty(\mathbb{S}^n_+)$ is equivalent to requiring that $\mathrm{RC}^* a_\alpha$ is a classical (i.e. one-step polyhomogeneous) symbol of order 0 on $\mathbb{R}^n$. This description also shows that the positive Euclidean Laplacian, Δ, is an element of $\mathrm{Diff}^2_{\mathrm{sc}}(\mathbb{S}^n_+)$. In terms of the 'inverted' polar coordinates on $\mathbb{R}^n$ we thus have that covectors $\xi \cdot dw$ take the form (3.4) with

$$\tau = -\frac{w \cdot \xi}{|w|} = -y \cdot \xi, \ \tau^2 + |\mu|^2 = |\xi|^2. \tag{3.6}$$

Here μ is the projection of ξ to the tangent space of the unit sphere $\mathbb{S}^{n-1}$ at $y \in \mathbb{S}^{n-1}$, and $|\mu|$ denotes the length of a covector on $\mathbb{S}^{n-1}$ with respect to the standard metric h on the unit sphere. In the general geometric setting, a similar identification can be made by first identifying X with $\mathbb{S}^n_+$ locally.

We next recall from [33] that polyhomogeneous symbols on X^a, pulled back to $\mathbb{R}^n$ by π^a, are smooth on the blown-up space $[\mathbb{S}^n_+; C_a]$. Recall that the (real) blow-up process is simply an invariant way of introducing polar coordinates about a submanifold. A full description appears in [18] and a more concise one in [19, Appendix A] and in [31]. In terms of the Euclidean variables, explicit local coordinates near the interior of the front face ff of the blow-up $[\mathbb{S}^n_+; C_a]$, i.e. near the interior of $\mathrm{ff} = \beta[\mathbb{S}^n_+; C_a]^* C_a$ are given by

(3.7)
$$x = |w_a|^{-1}, \ y_j = \frac{(w_a)_j}{|w_a|} \ (j = 1, \ldots, m-1), \ Z_j = (w^a)_j \ (j = 1, \ldots, n-m).$$

Similarly, one can easily write down local coordinates near the corner $\mathrm{ff} \cap \beta[\mathbb{S}^n_+; C_a]^* C_0$, $C_0 = \mathbb{S}^{n-1}$, see [31, Section 2]. As a result of such calculations, we conclude that if $V_a \in S^{-1}_{\mathrm{phg}}(X^a)$, i.e. $V_a \in x_a \mathcal{C}^\infty(\bar{X}_a)$, then $(\pi^a)^* V_a \in \mathcal{C}^\infty([\mathbb{S}^n_+; C_a])$, vanishing at the free face, i.e. the lift, $\beta[\mathbb{S}^n_+; C_a]^* C_0$, of $C_0 = \mathbb{S}^{n-1}$ (we dropped pull-back by RC^{-1} as well as the blow-down map in the notation; we drop $(\pi^a)^*$ presently as well).

Thus, for a Euclidean many-body Hamiltonian, $H = \Delta + \sum_a V_a$, V_a becomes a smooth function on the compact resolved space $[\mathbb{S}^n_+; C_a]$. Hence, to understand H, we need to blow up *all* the C_a. The iterative construction was carried out in detail in [31, Section 2]; we refer to the discussion given there for details. However, we remind the reader that the C_a are blown up in the order of inclusion (*opposite* to the usual order on the clusters). That is, one starts with the blow-up of 2-clusters (which are disjoint); 3-clusters become disjoint upon this blow-up. One proceeds to blow-up the 3-clusters; 4-clusters become disjoint now. One proceeds this way, finally blowing up the $N-1$-clusters. (The blow-up of the N-cluster is a diffeomorphism, hence can be neglected.) We thus obtain a manifold with corners which is denoted by $[\mathbb{S}^n_+;\mathcal{C}]$.

More generally, we can let X be a compact manifold with boundary (in place of $\mathbb{S}^n_+$), and let

$$\mathcal{C} = \{C_a : \ a \in I\} \tag{3.8}$$

be a finite set of closed embedded submanifolds of ∂X such that $\partial X = C_0 \in \mathcal{C}$ and for all $a, b \in I$ either C_a and C_b are disjoint, or they intersect cleanly and $C_a \cap C_b = C_c$ for some $c \in I$. Then $[X;\mathcal{C}]$ can be defined via a series of blow-ups as above.

The algebra of many-body differential operators is then defined as

$$\mathrm{Diff}_{\mathrm{Sc}}(X,\mathcal{C}) = \mathcal{C}^\infty([X;\mathcal{C}]) \otimes_{\mathcal{C}^\infty(X)} \mathrm{Diff}_{\mathrm{sc}}(X). \tag{3.9}$$

That is, similarly to (3.5), $P \in \mathrm{Diff}^m_{\mathrm{Sc}}(\mathbb{S}^n_+,\mathcal{C})$ means that

$$P = \sum_{|\alpha|\leq m} a_\alpha D^\alpha_w, \quad a_\alpha \in \mathcal{C}^\infty([\mathbb{S}^n_+;\mathcal{C}]) \tag{3.10}$$

where we again ignored the pull-back by RC in the notation. The Euclidean many-body Hamiltonian H is thus in $\mathrm{Diff}^2_{\mathrm{Sc}}(\mathbb{S}^n_+,\mathcal{C})$.

One of the main differences between $\mathrm{Diff}_{\mathrm{Sc}}(X,\mathcal{C})$ and $\mathrm{Diff}_{\mathrm{sc}}(X)$ is that the former is not commutative to 'top weight'. That is, while for $P \in \mathrm{Diff}^m_{\mathrm{sc}}(X)$, $Q \in \mathrm{Diff}^{m'}_{\mathrm{sc}}(X)$, we have $[P,Q] \in x\,\mathrm{Diff}^{m+m'-1}_{\mathrm{sc}}(X)$, this is replaced by $[P,Q] \in \rho_{C_0}\,\mathrm{Diff}^{m+m'-1}_{\mathrm{Sc}}(X,\mathcal{C})$ for $P \in \mathrm{Diff}^m_{\mathrm{Sc}}(X,\mathcal{C})$, $Q \in \mathrm{Diff}^{m'}_{\mathrm{Sc}}(X,\mathcal{C})$ with ρ_{C_0} a defining function for the lift of C_0. Thus, a vanishing factor (such as x above) is only present at the lift of the free face C_0, i.e. there is no gain of a weight factor at the front faces ff.

Now consider the operator $H = \Delta + V$, $V \in \mathcal{C}^\infty([X;\mathcal{C}])$ vanishing at the free face (the lift of C_0), discussed above. As indicated in the previous paragraph, for $P \in \mathrm{Diff}^m_{\mathrm{sc}}(X)$,

$$[\Delta, P] \in x\,\mathrm{Diff}^{m+1}_{\mathrm{sc}}(X) \subset x\,\mathrm{Diff}^{m+1}_{\mathrm{Sc}}(X,\mathcal{C}). \tag{3.11}$$

On the other hand,

$$[V, P] \in \rho^2_{C_0}\,\mathrm{Diff}^{m-1}_{\mathrm{Sc}}(X,\mathcal{C}). \tag{3.12}$$

Hence, as expected, $[V,P]$ is lower order than $[\Delta,P]$ at the lift of C_0, but 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, in our Euclidean setting, we take $P \in \mathrm{Diff}_{\mathrm{sc}}(\mathbb{S}^n_+)$ as in (3.5), so $a_\alpha \in \mathcal{C}^\infty(\mathbb{S}^n_+)$, and such that $a_\alpha|_{C_a} = 0$ unless only derivatives with respect to the external variables, $D_{(w_a)^j}$ appear in D^α. That is, writing the full symbol of P as a polynomial on ${}^{\mathrm{sc}}T^*\mathbb{S}^n_+$, namely $p = \sum_{|\alpha|\leq m} a_\alpha \xi^\alpha$, we require that p is π-invariant, i.e. $p|_{{}^{\mathrm{sc}}T^*_{C_a}\mathbb{S}^n_+}$ is independent of

ξ^a. This makes $[V, P]$ the same order as $[\Delta, P]$ with additional vanishing at the lift of C_0 which will be sufficient for the commutator arguments. Indeed, the standard Poisson bracket formula lets us compute $[H, P]$ to 'top weight' at the lift of C_0, and then a compactness argument, based on those of Froese and Herbst [5], described in the introduction, allows us to obtain a positivity estimate at all boundary faces of $[\mathbb{S}^n_+; \mathcal{C}]$ (or $[X; \mathcal{C}]$ in general). It is the π-invariance of p (and the corresponding statement in the pseudo-differential setting) that allows microlocalization only in the compressed bundle, ${}^{\mathrm{sc}}\dot{T}^*\mathbb{S}^n_+$, not in ${}^{\mathrm{sc}}T^*\mathbb{S}^n_+$.

To prove the propagation estimates, we need to microlocalize such arguments, i.e. employ the many-body pseudo-differential calculus developped in [31]. Rather than developing this in detail here, we just mention that our positive commutator estimates rely on operators that are essentially quantizations of π-invariant functions on ${}^{\mathrm{sc}}T^*\mathbb{S}^n_+$, much as outlined above for differential operators. Such operators would be in Melrose's scattering calculus, were it not for the non-symbolic behavior as $\xi \to \infty$ that the π-invariance imposes on non-polynomial functions. To eliminate the inconvenient behavior as $\xi \to \infty$ we compose the operator with $\psi(H)$, $\psi \in \mathcal{C}^\infty_c(\mathbb{R})$ supported near λ; the result is indeed an operator A in the many-body pseudo-differential calculus. The positive commutator proofs will then rely on the construction of π-invariant functions on ${}^{\mathrm{sc}}T^*\mathbb{S}^n_+$ with positive derivative along the Hamilton vector fields ${}^{\mathrm{sc}}H^b_g$ in the relevant part of phase space (cf. Definition 2.1), and then proving that $i[\psi_0(H)A^*A\psi_0(H), H]$ is positive modulo lower order terms in the appropriate part of phase space for ψ_0 of sufficiently small support near λ. This part of the proof is analogous to that of Froese and Herbst [5] as outlined in the introduction; it is an inductive argument showing that the various indicial operators of the commutator are positive (without compact errors!).

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